

# Covariance Functions for Multivariate Gaussian Fields evolving temporally over Planet Earth

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## Abstract

The construction of valid and flexible cross-covariance functions is a fundamental task for modelling multivariate space-time data arising from climatological and oceanographical phenomena. Indeed, a suitable specification of the covariance structure allows to capture both the space-time dependencies between the observations and the development of accurate predictions. For data observed over large portions of planet Earth it is necessary to take into account the curvature of the planet. Hence the need for random field models defined over spheres across time. In particular, the associated covariance function should depend on the geodesic distance, which is the most natural metric over the spherical surface. In this work, we provide a complete characterisation for the space-time cross-covariances, that are continuous, geodesically isotropic in the spatial variable and stationary in the temporal one, and discuss some fundamentals and construction principles of matrix-valued covariances on spheres. We propose a flexible parametric family of matrix-valued covariance functions, with both marginal and cross structure being of the Gneiting type. We additionally introduce a different multivariate Gneiting model based on the adaptation of the latent dimension approach to the spherical context. Finally, we assess the performance of our models through simulation experiments, and we analyse a bivariate space-time data set of surface air temperatures and atmospheric pressures.

*Keywords:* Atmospheric pressure; Geodesic; Gneiting classes; Latent dimensions; Space-time; Sphere; Temperature.

# 1 Introduction

Monitoring several georeferenced variables is a common practice in a wide range of disciplines such as climatology and oceanography. The phenomena under study are often observed over large portions of the Earth and across several time instants. Since there is only a finite sample from the involved variables, geostatistical models are a useful tool to capture both the spatial and temporal interactions between the observed data, as well as the uncertainty associated to the limited available information (Cressie, 1993; Wackernagel, 2003; Gneiting et al., 2007). The geostatistical approach consists in modelling the observations as a partial realisation of a space-time multivariate random field (RF), denoted as

$$\{\mathbf{Z}(\mathbf{x}, t) = (Z_1(\mathbf{x}, t), \dots, Z_m(\mathbf{x}, t))^{\top} : (\mathbf{x}, t) \in \mathcal{D} \times \mathcal{T}\},$$

where  $\top$  is the transpose operator and  $m$  is a positive integer representing the number of components of the field. If  $m = 1$ , we say that  $Z$  is a univariate (or scalar-valued) random field, whereas for  $m > 1$ ,  $\mathbf{Z}$  is called an  $m$ -variate (or vector-valued) random field. Here,  $\mathcal{D}$  and  $\mathcal{T}$  denote the spatial and temporal domains, respectively. Throughout, we assume that  $\mathbf{Z}$  is Gaussian, so that a suitable specification of the covariance structure of  $\mathbf{Z}$  is crucial to develop both accurate inferences and predictions over unobserved sites (Cressie, 1993).

Matrix-valued covariance functions are typically given in terms of Euclidean distances. The literature for this case is extensive and we refer the reader to the review by Genton and Kleiber (2015) with the references therein. The main motivation to consider the Euclidean metric is the existence of several methods for projecting the geographical coordinates, longitude and latitude, onto the plane. However, when a phenomenon is observed over the whole planet Earth, the approach based on projections generates apparent distortions in the distances associated to distant locations on the globe. The reader is referred to Banerjee (2005), where the impact of the different types of projections with respect to spatial inference is discussed. Indeed, the geometry of the Earth must be considered. Thus, it is more realistic to work under the framework of random fields defined spatially on a sphere (see Marinucci and Peccati, 2011).

Let  $d$  be a positive integer. The  $d$ -dimensional unit sphere is denoted as  $\mathbb{S}^d := \{\mathbf{x} \in \mathbb{R}^{d+1} : \|\mathbf{x}\| = 1\}$ , where  $\|\cdot\|$  represents the Euclidean norm. The most accurate metric in the spherical scenario is the geodesic (or great circle) distance, which roughly speaking corresponds to the arc joining any two points located on the sphere, measured along a path on the spherical surface. Formally, the geodesic

distance is defined as the mapping  $\theta : \mathbb{S}^d \times \mathbb{S}^d \rightarrow [0, \pi]$  given by

$$\theta := \theta(\mathbf{x}, \mathbf{y}) = \arccos(\mathbf{x}^\top \mathbf{y}).$$

The construction of valid and flexible covariance functions in terms of the geodesic distance is a challenging problem and requires the application of the theory of positive definite functions on spheres (Schoenberg, 1942; Yaglom, 1987; Hannan, 2009; Berg and Porcu, 2016). In the univariate and merely spatial case, Huang et al. (2011) study the validity of some specific covariance functions. The essay by Gneiting (2013) contains a wealth of results related to the validity of a wide range of covariance families. Other related works are the study of star-shaped random particles (Hansen et al., 2011) and convolution roots (Ziegel, 2014). However, the spatial and spatio-temporal covariances in the multivariate case are still unexplored, with the works of Berg and Porcu (2016) and Porcu et al. (2016) being notable exceptions.

In this work, we propose some progress in this area. First, we give a complete characterisation for the space-time matrix-valued covariances, being continuous, geodesically isotropic in the spatial variable and stationary in the temporal one. Our characterisation generalises to the multivariate case the result given by Berg and Porcu (2016). Also, we discuss several interesting aspects, such as different notions of separability and some construction principles, of cross-covariances on  $\mathbb{S}^d \times \mathbb{R}$ .

The Gneiting class (Gneiting, 2002) is one of the most popular space-time covariance families and some adaptations in terms of geodesic distance have been given by Porcu et al. (2016). We extend to the multivariate scenario the modified Gneiting class introduced by Porcu et al. (2016). Furthermore, we adapt to the spherical context the latent dimension approach (Apanasovich and Genton, 2010) and we then generate additional Gneiting type matrix-valued covariances. The proposed models are non-separable with respect to the components of the field nor with respect to the space-time interactions. To obtain these results, we have demonstrated several technical results that can be useful to develop new research in this area.

Our findings are illustrated through simulation studies as well as a real data application. In particular, we analyse a bivariate space-time data set of surface air temperatures and atmospheric pressures. These variables have been generated from the Community Climate System Model (CCSM) provided by NCAR (National Center for Atmospheric Research). We compare the performance of the proposed models to the traditional linear model of coregionalisation.

The remainder of the article is organised as follows. Section 2 introduces the main notation and some preliminary results on positive definite functions. In Section 3, we give a characterisation for the space-time matrix-valued covariance functions, defined spatially in terms of the geodesic distance. Some fundamentals of space-time cross-covariances on spheres are additionally discussed. Section 4 provides some multivariate Gneiting type families. In order to illustrate the properties of the proposed models, Section 5 contains simulation experiments and a real data example of surface air temperatures and atmospheric pressures.

## 2 Background

This section introduces the main notation and preliminaries of the paper. We start with positive definite functions, that arise in statistics as the covariances of Gaussian random fields as well as the characteristic functions of probability distributions.

**Definition 2.1.** Let  $\mathcal{E}$  be a non-empty set and  $m \in \mathbb{N}$ . We say that the matrix-valued function  $\mathbf{F} : \mathcal{E} \times \mathcal{E} \rightarrow \mathbb{R}^{m \times m}$  is positive definite if for all integer  $n \geq 1$ ,  $\{e_1, \dots, e_n\} \subset \mathcal{E}$  and  $\{\mathbf{a}_1, \dots, \mathbf{a}_n\} \subset \mathbb{R}^m$ , the following inequality holds:

$$\sum_{\ell=1}^n \sum_{r=1}^n \mathbf{a}_\ell^\top \mathbf{F}(e_\ell, e_r) \mathbf{a}_r \geq 0. \quad (2.1)$$

We denote as  $\mathcal{P}^m(\mathcal{E})$  the class of such mappings  $\mathbf{F}$  satisfying (2.1).

Next, we focus on the cases where  $\mathcal{E}$  is either  $\mathbb{R}^d$ ,  $\mathbb{S}^d$  or  $\mathbb{S}^d \times \mathbb{R}^k$ , for  $d, k \in \mathbb{N}$ . For a clear presentation of the results, Table 2.1 summarises the notation introduced along the paper.

### 2.1 Matrix-valued positive definite functions on Euclidean spaces

This section provides a brief review about matrix-valued positive definite functions on the Euclidean space  $\mathcal{E} = \mathbb{R}^d$ . Specifically, we expose some characterisations for the stationary and Euclidean isotropic members of the class  $\mathcal{P}^m(\mathbb{R}^d)$ .

Table 2.1: Summary of the notation used along the paper. Throughout, in the univariate case ( $m = 1$ ) we omit the super index:  $\mathcal{P}(\mathcal{E})$ ,  $\Phi_{d,\mathcal{S}}$ ,  $\Phi_{d,\mathcal{I}}$ ,  $\Psi_{d,\mathcal{I}}$  and  $\Upsilon_{d,k}$  are used instead of  $\mathcal{P}^1(\mathcal{E})$ ,  $\Phi_{d,\mathcal{S}}^1$ ,  $\Phi_{d,\mathcal{I}}^1$ ,  $\Psi_{d,\mathcal{I}}^1$  and  $\Upsilon_{d,k}^1$ , respectively.

Notation	Description
$\mathcal{P}^m(\mathcal{E})$	Positive definite matrix-valued $(m \times m)$ functions on $\mathcal{E} \times \mathcal{E}$ .
$\Phi_{d,\mathcal{S}}^m$	Continuous, bounded and stationary elements of $\mathcal{P}^m(\mathbb{R}^d)$ .
$\Phi_{d,\mathcal{I}}^m$	Continuous, bounded and Euclidean isotropic elements of $\mathcal{P}^m(\mathbb{R}^d)$ .
$\Psi_{d,\mathcal{I}}^m$	Continuous, bounded and geodesically isotropic elements of $\mathcal{P}^m(\mathbb{S}^d)$ .
$\Upsilon_{d,k}^m$	Elements in $\mathcal{P}^m(\mathbb{S}^d \times \mathbb{R}^k)$ being, continuous, bounded, geodesically isotropic in the spherical variable and stationary in the Euclidean variable.

### Stationarity: the class $\Phi_{d,\mathcal{S}}^m$

We say that  $\mathbf{F} \in \mathcal{P}^m(\mathbb{R}^d)$  is stationary if there exists a mapping  $\tilde{\varphi} : \mathbb{R}^d \rightarrow \mathbb{R}^{m \times m}$  such that

$$\mathbf{F}(\mathbf{x}, \mathbf{y}) = \tilde{\varphi}(\mathbf{x} - \mathbf{y}) = [\tilde{\varphi}_{ij}(\mathbf{x} - \mathbf{y})]_{i,j=1}^m, \quad \mathbf{x}, \mathbf{y} \in \mathbb{R}^d. \quad (2.2)$$

We call  $\Phi_{d,\mathcal{S}}^m$  the class of continuous mappings  $\tilde{\varphi}$  such that  $\mathbf{F}$  in (2.2) is positive definite. Cramér's Theorem (Cramer, 1940) establishes that  $\tilde{\varphi} \in \Phi_{d,\mathcal{S}}^m$  if and only if it can be represented through

$$\tilde{\varphi}(\mathbf{h}) = \int_{\mathbb{R}^d} \exp\{\imath \mathbf{h}^\top \boldsymbol{\omega}\} d\tilde{\Lambda}_d(\boldsymbol{\omega}), \quad \mathbf{h} \in \mathbb{R}^d, \quad (2.3)$$

where  $\imath = \sqrt{-1} \in \mathbb{C}$  and  $\tilde{\Lambda}_d : \mathbb{R}^d \rightarrow \mathbb{C}^{m \times m}$  is a matrix-valued mapping, with increments being Hermitian and positive definite matrices, and whose elements,  $\tilde{\Lambda}_{d,ij}(\cdot)$ , for  $i, j = 1, \dots, m$ , are functions of bounded variation (see Wackernagel, 2003). In particular, the diagonal terms,  $\tilde{\Lambda}_{d,ii}(\boldsymbol{\omega})$ , are real, non-decreasing and bounded, whereas the off-diagonal elements are generally complex-valued. Cramer's Theorem is the multivariate version of the celebrated Bochner's Theorem (Bochner, 1955). If the elements of  $\tilde{\Lambda}_d(\cdot)$  are absolutely continuous, then Equation (2.3) simplifies to

$$\tilde{\varphi}(\mathbf{h}) = \int_{\mathbb{R}^d} \exp\{\imath \mathbf{h}^\top \boldsymbol{\omega}\} \tilde{\lambda}_d(\boldsymbol{\omega}) d\boldsymbol{\omega}, \quad \mathbf{h} \in \mathbb{R}^d,$$

with  $\tilde{\lambda}_d(\boldsymbol{\omega}) = [\tilde{\lambda}_{d,ij}(\boldsymbol{\omega})]_{i,j=1}^m$  being Hermitian and positive definite, for any  $\boldsymbol{\omega} \in \mathbb{R}^d$ . The mapping  $\tilde{\lambda}_d(\boldsymbol{\omega})$  is known as the matrix-valued *spectral density* and classical Fourier inversion yields

$$\tilde{\lambda}_d(\boldsymbol{\omega}) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \exp\{-\imath \mathbf{h}^\top \boldsymbol{\omega}\} \tilde{\varphi}(\mathbf{h}) d\mathbf{h}, \quad \boldsymbol{\omega} \in \mathbb{R}^d.$$

Finally, the following inequality between the elements of  $\tilde{\varphi}$  is true

$$|\tilde{\varphi}_{ij}(\mathbf{h})|^2 \leq \tilde{\varphi}_{ii}(\mathbf{0})\tilde{\varphi}_{jj}(\mathbf{0}), \quad \text{for all } \mathbf{h} \in \mathbb{R}^d.$$

However, the maximum value of the mapping  $\tilde{\varphi}_{ij}(\mathbf{h})$ , with  $i \neq j$ , is not necessarily reached at  $\mathbf{h} = \mathbf{0}$ . In general,  $\tilde{\varphi}_{ij}$  is not itself a scalar-valued positive definite function when  $i \neq j$ .

### Euclidean isotropy: the class $\Phi_{d,\mathcal{I}}^m$

Consider an element  $\mathbf{F}$  in  $\mathcal{P}^m(\mathbb{R}^d)$  and suppose that there exists a continuous and bounded mapping  $\varphi : \mathbb{R}_+ \rightarrow \mathbb{R}^{m \times m}$  such that

$$\mathbf{F}(\mathbf{x}, \mathbf{y}) = \varphi(\|\mathbf{x} - \mathbf{y}\|), \quad \mathbf{x}, \mathbf{y} \in \mathbb{R}^d.$$

Then,  $\mathbf{F}$  is called stationary and *Euclidean isotropic* (or radial). We denote as  $\Phi_{d,\mathcal{I}}^m$  the class of bounded, continuous, stationary and Euclidean isotropic mappings  $\varphi(\cdot) = [\varphi_{ij}(\cdot)]_{i,j=1}^m$ .

When  $m = 1$ , characterisation of the class  $\Phi_{d,\mathcal{I}}$  was provided through the celebrated paper by [Schoenberg \(1938\)](#). [Alonso-Malaver et al. \(2015\)](#) characterise the class  $\Phi_{d,\mathcal{I}}^m$  through the continuous members  $\varphi$  having representation

$$\varphi(r) = \int_{[0,\infty)} \Omega_d(r\omega) d\mathbf{\Lambda}_d(\omega), \quad r \geq 0,$$

where  $\mathbf{\Lambda}_d : [0, \infty) \rightarrow \mathbb{R}^{m \times m}$  is a matrix-valued mapping, with increments being positive definite matrices, and elements  $\Lambda_{d,ij}(\cdot)$  of bounded variation, for each  $i, j = 1, \dots, m$ . Here, the function  $\Omega_d(\cdot)$  is defined as

$$\Omega_d(z) = \Gamma(d/2)(z/2)^{-(d-2)/2} J_{(d-2)/2}(z), \quad z \geq 0,$$

with  $\Gamma$  being the Gamma function and  $J_\nu$  the Bessel function of the first kind of degree  $\nu$  (see [Abramowitz and Stegun, 1970](#)). If the elements of  $\mathbf{\Lambda}_d(\cdot)$  are absolutely continuous, then we have an associated spectral density  $\boldsymbol{\lambda}_d : [0, \infty) \rightarrow \mathbb{R}^{m \times m}$  as in the stationary case, which is called, following [Daley and Porcu \(2014\)](#), a  $d$ -Schoenberg matrix.

The classes  $\Phi_{d,\mathcal{I}}^m$  are non-increasing in  $d$ , and the following inclusion relations are strict

$$\Phi_{\infty,\mathcal{I}}^m := \bigcap_{d=1}^{\infty} \Phi_{d,\mathcal{I}}^m \subset \dots \subset \Phi_{2,\mathcal{I}}^m \subset \Phi_{1,\mathcal{I}}^m.$$

The elements  $\varphi$  in the class  $\Phi_{\infty, \mathcal{I}}^m$  can be represented as

$$\varphi(r) = \int_{[0, \infty)} \exp(-r^2 \omega^2) d\mathbf{\Lambda}(\omega), \quad r \geq 0,$$

where  $\mathbf{\Lambda}$  is a matrix-valued mapping with similar properties as  $\mathbf{\Lambda}_d$ .

## 2.2 Matrix-valued positive definite functions on $\mathbb{S}^d$ and the class $\Psi_{d, \mathcal{I}}^m$

In this section, we pay attention to matrix-valued positive definite functions on the unit sphere. Consider  $\mathbf{F} = [F_{ij}]_{i,j=1}^m \in \mathcal{P}^m(\mathbb{S}^d)$ . We say that  $\mathbf{F}$  is *geodesically isotropic* if there exists a bounded and continuous mapping  $\psi : [0, \pi] \rightarrow \mathbb{R}^{m \times m}$  such that

$$\mathbf{F}(\mathbf{x}, \mathbf{y}) = \psi(\theta(\mathbf{x}, \mathbf{y})), \quad \mathbf{x}, \mathbf{y} \in \mathbb{S}^d.$$

The continuous mappings  $\psi$  are the elements of the class  $\Psi_{d, \mathcal{I}}^m$  and the following inclusion relations are true:

$$\Psi_{\infty, \mathcal{I}}^m = \bigcap_{d=1}^{\infty} \Psi_{d, \mathcal{I}}^m \subset \cdots \subset \Psi_{2, \mathcal{I}}^m \subset \Psi_{1, \mathcal{I}}^m, \quad (2.4)$$

where  $\Psi_{\infty, \mathcal{I}}^m$  is the class of geodesically isotropic positive definite functions being valid on the Hilbert sphere  $\mathbb{S}^\infty = \{(x_n)_{n \in \mathbb{N}} \in \mathbb{R}^\mathbb{N} : \sum_{n \in \mathbb{N}} x_n^2 = 1\}$ .

The elements of the class  $\Psi_{d, \mathcal{I}}^m$  have an explicit connection with Gegenbauer (or ultraspherical) polynomials (Abramowitz and Stegun, 1970). Here,  $\mathcal{G}_n^\lambda$  denotes the  $\lambda$ -Gegenbauer polynomial of degree  $n$ , which is defined implicitly through the expression

$$\frac{1}{(1 + r^2 - 2r \cos \theta)^\lambda} = \sum_{n=0}^{\infty} r^n \mathcal{G}_n^\lambda(\cos \theta), \quad \theta \in [0, \pi], \quad r \in (-1, 1).$$

In particular,  $\mathcal{T}_n := \mathcal{G}_n^0$  and  $\mathcal{P}_n := \mathcal{G}_n^{1/2}$  are respectively the Chebyshev and Legendre polynomials of degree  $n$ .

The following result (Hannan, 2009; Yaglom, 1987) offers a complete characterisation of the classes  $\Psi_{d, \mathcal{I}}^m$  and  $\Psi_{\infty, \mathcal{I}}^m$ , and corresponds to the multivariate version of Schoenberg's Theorem (Schoenberg, 1942). Equalities and summability conditions for matrices must be understood in a componentwise sense.

**Theorem 2.1.** Let  $d$  and  $m$  be positive integers.

(1) The mapping  $\psi$  is a member of the class  $\Psi_{d,\mathcal{I}}^m$  if and only if it admits the representation

$$\psi(\theta) = \sum_{n=0}^{\infty} \mathbf{B}_{n,d} \frac{\mathcal{G}_n^{(d-1)/2}(\cos \theta)}{\mathcal{G}_n^{(d-1)/2}(1)}, \quad \theta \in [0, \pi], \quad (2.5)$$

where  $\{\mathbf{B}_{n,d}\}_{n=0}^{\infty}$  is a sequence of symmetric, positive definite and summable matrices.

(2) The mapping  $\psi$  is a member of the class  $\Psi_{\infty,\mathcal{I}}^m$  if and only if it can be represented as

$$\psi(\theta) = \sum_{n=0}^{\infty} \mathbf{B}_n (\cos \theta)^n, \quad \theta \in [0, \pi],$$

where  $\{\mathbf{B}_n\}_{n=0}^{\infty}$  is a sequence of symmetric, positive definite and summable matrices.

Using orthogonality properties of Gegenbauer polynomials ([Abramowitz and Stegun, 1970](#)) and through classical Fourier inversion we can prove that

$$\begin{aligned} \mathbf{B}_{0,1} &= \frac{1}{\pi} \int_0^\pi \psi(\theta) d\theta, \\ \mathbf{B}_{n,1} &= \frac{2}{\pi} \int_0^\pi \cos(n\theta) \psi(\theta) d\theta, \quad \text{for } n \geq 1, \end{aligned} \quad (2.6)$$

whereas for  $d \geq 2$ , we have

$$\mathbf{B}_{n,d} = \frac{(2n+d-1)}{2^{3-d}\pi} \frac{[\Gamma((d-1)/2)]^2}{\Gamma(d-1)} \int_0^\pi \mathcal{G}_n^{(d-1)/2}(\cos \theta) (\sin \theta)^{d-1} \psi(\theta) d\theta, \quad n \geq 0, \quad (2.7)$$

where integration is taken componentwise. The matrices  $\{\mathbf{B}_{n,d}\}_{n=0}^{\infty}$  are called *Schoenberg's matrices*. For the case  $m = 1$ , such result is reported by [Gneiting \(2013\)](#).

### 2.3 Scalar-valued positive definite functions on $\mathbb{S}^d \times \mathbb{R}^k$ and the class $\Upsilon_{d,k}$

Now, we consider the class of scalar-valued positive definite functions on  $\mathbb{S}^d \times \mathbb{R}^k$ , for  $d, k \in \mathbb{N}$ . Particularly, we focus on those continuous elements being geodesically isotropic in the spherical component and stationary in the Euclidean one. Suppose that  $F$  is a member of the class  $\mathcal{P}(\mathbb{S}^d \times \mathbb{R}^k)$  and there exists a bounded and continuous mapping  $C : [0, \pi] \times \mathbb{R}^k \rightarrow \mathbb{R}$  such that

$$F((\mathbf{x}, \mathbf{t}), (\mathbf{y}, \mathbf{s})) = C(\theta(\mathbf{x}, \mathbf{y}), \mathbf{t} - \mathbf{s}), \quad \mathbf{x}, \mathbf{y} \in \mathbb{S}^d, \mathbf{t}, \mathbf{s} \in \mathbb{R}^k. \quad (2.8)$$



The continuous mappings  $C$  such that  $F$  in (2.8) is positive definite are the elements of the class  $\Upsilon_{d,k}$ . These classes are non-increasing in  $d$  and we have the inclusions

$$\Upsilon_{\infty,k} := \bigcap_{d=1}^{\infty} \Upsilon_{d,k} \subset \cdots \subset \Upsilon_{2,k} \subset \Upsilon_{1,k}.$$

The following theorem given by [Berg and Porcu \(2016\)](#) characterises completely the classes  $\Upsilon_{d,k}$  and  $\Upsilon_{\infty,k}$ .

**Theorem 2.2.** Let  $d$  and  $k$  be positive integers and  $C : [0, \pi] \times \mathbb{R}^k \rightarrow \mathbb{R}$  a continuous mapping, with  $C(0, \mathbf{0}) < \infty$ .

(1) The mapping  $C$  belongs to the class  $\Upsilon_{d,k}$  if and only if it can be represented as

$$C(\theta, \mathbf{u}) = \sum_{n=0}^{\infty} \tilde{\varphi}_{n,d}(\mathbf{u}) \frac{\mathcal{G}_n^{(d-1)/2}(\cos \theta)}{\mathcal{G}_n^{(d-1)/2}(1)}, \quad (\theta, \mathbf{u}) \in [0, \pi] \times \mathbb{R}^k, \quad (2.9)$$

where  $\{\tilde{\varphi}_{n,d}(\cdot)\}_{n=0}^{\infty}$  is a sequence of elements in  $\Phi_{k,\mathcal{S}}$ , such that  $\sum_{n=0}^{\infty} \tilde{\varphi}_{n,d}(\mathbf{0}) < \infty$ .

(2) The mapping  $C$  belongs to the class  $\Upsilon_{\infty,k}$  if and only if it admits the representation

$$C(\theta, \mathbf{u}) = \sum_{n=0}^{\infty} \tilde{\varphi}_n(\mathbf{u}) (\cos \theta)^n, \quad (\theta, \mathbf{u}) \in [0, \pi] \times \mathbb{R}^k, \quad (2.10)$$

where  $\{\tilde{\varphi}_n(\cdot)\}_{n=0}^{\infty}$  is a sequence of elements in  $\Phi_{k,\mathcal{S}}$ , with  $\sum_{n=0}^{\infty} \tilde{\varphi}_n(\mathbf{0}) < \infty$ .

**Remark 2.1.** The result given by [Berg and Porcu \(2016\)](#) is more general, since  $\mathbb{R}^k$  can be replaced for any locally compact group.

The orthogonality of Gegenbauer polynomials ([Abramowitz and Stegun, 1970](#)) implies that

$$\begin{aligned} \tilde{\varphi}_{0,1}(\mathbf{u}) &= \frac{1}{\pi} \int_0^\pi C(\theta, \mathbf{u}) d\theta, \\ \tilde{\varphi}_{n,1}(\mathbf{u}) &= \frac{2}{\pi} \int_0^\pi \cos(n\theta) C(\theta, \mathbf{u}) d\theta, \quad \text{for } n \geq 1, \end{aligned} \quad (2.11)$$

whereas for  $d \geq 2$ ,

$$\tilde{\varphi}_{n,d}(\mathbf{u}) = \frac{(2n+d-1)}{2^{3-d}\pi} \frac{[\Gamma((d-1)/2)]^2}{\Gamma(d-1)} \int_0^\pi \mathcal{G}_n^{(d-1)/2}(\cos \theta) (\sin \theta)^{d-1} C(\theta, \mathbf{u}) d\theta, \quad n \geq 0. \quad (2.12)$$

[Berg and Porcu \(2016\)](#) call the sequence of mappings  $\{\tilde{\varphi}_{n,d}(\cdot)\}_{n=0}^{\infty}$  as *Schoenberg's functions*.

### 3 Space-time cross-covariances for RFs defined on spheres across time

Let  $d$ ,  $k$  and  $m$  be positive integers. We now study the class of matrix-valued positive definite functions on  $\mathbb{S}^d \times \mathbb{R}^k$ , being bounded, continuous, geodesically isotropic in the spherical component and stationary in the Euclidean one. The case  $k = 1$  is particularly important, since  $\mathcal{P}^m(\mathbb{S}^d \times \mathbb{R})$  can be interpreted as the class of admissible space-time covariances for multivariate Gaussian RFs, with spatial locations on the unit sphere. However, the main result of this section, given in Theorem 3.1 is provided for an arbitrary  $k \in \mathbb{N}$ , since we require this general framework in the coming sections, as it will become apparent subsequently.

#### 3.1 Matrix-valued positive definite functions on $\mathbb{S}^d \times \mathbb{R}^k$ : the class $\Upsilon_{d,k}^m$ and its characterisation

Consider  $\mathbf{F} \in \mathcal{P}^m(\mathbb{S}^d \times \mathbb{R}^k)$  and suppose that there exists a bounded and continuous mapping  $\mathbf{C} : [0, \pi] \times \mathbb{R}^k \rightarrow \mathbb{R}^{m \times m}$  such that

$$\mathbf{F}((\mathbf{x}, \mathbf{t}), (\mathbf{y}, \mathbf{s})) = \mathbf{C}(\theta(\mathbf{x}, \mathbf{y}), \mathbf{t} - \mathbf{s}), \quad \mathbf{x}, \mathbf{y} \in \mathbb{S}^d, \mathbf{t}, \mathbf{s} \in \mathbb{R}^k. \quad (3.1)$$

Such mappings  $\mathbf{C}$  are the elements of the class  $\Upsilon_{d,k}^m$ . These classes are non-increasing in  $d$  and we have the inclusions

$$\Upsilon_{\infty,k}^m := \bigcap_{d=1}^{\infty} \Upsilon_{d,k}^m \subset \cdots \subset \Upsilon_{2,k}^m \subset \Upsilon_{1,k}^m.$$

Now, we propose the generalisation of Theorem 2.2 to the multivariate case. Theorem 3.1 offers a complete characterisation of the class  $\Upsilon_{d,k}^m$  and  $\Upsilon_{\infty,k}^m$ , for any  $m \geq 1$ . Again, equalities and summability conditions must be understood in a componentwise sense.

**Theorem 3.1.** Let  $d$ ,  $k$  and  $m$  be positive integers and  $\mathbf{C} : [0, \pi] \times \mathbb{R}^k \rightarrow \mathbb{R}^{m \times m}$  a continuous matrix-valued mapping, with  $C_{ii}(0, \mathbf{0}) < \infty$ , for all  $i = 1, \dots, m$ .

(1) The mapping  $\mathbf{C}$  belongs to the class  $\Upsilon_{d,k}^m$  if and only if

$$\mathbf{C}(\theta, \mathbf{u}) = \sum_{n=0}^{\infty} \tilde{\varphi}_{n,d}(\mathbf{u}) \frac{\mathcal{G}_n^{(d-1)/2}(\cos \theta)}{\mathcal{G}_n^{(d-1)/2}(1)}, \quad (\theta, \mathbf{u}) \in [0, \pi] \times \mathbb{R}^k, \quad (3.2)$$

with  $\{\tilde{\varphi}_{n,d}(\cdot)\}_{n=0}^{\infty}$  being a sequence of members of the class  $\Phi_{k,\mathcal{S}}^m$ , with the additional requirement that the sequence of matrices  $\{\tilde{\varphi}_{n,d}(\mathbf{0})\}_{n=0}^{\infty}$  is summable.

(2) The mapping  $\mathbf{C}$  belongs to the class  $\Upsilon_{\infty,k}^m$  if and only if

$$\mathbf{C}(\theta, \mathbf{u}) = \sum_{n=0}^{\infty} \tilde{\varphi}_n(\mathbf{u})(\cos \theta)^n, \quad (\theta, \mathbf{u}) \in [0, \pi] \times \mathbb{R}^k, \quad (3.3)$$

with  $\{\tilde{\varphi}_n(\cdot)\}_{n=0}^{\infty}$  being a sequence of members of the class  $\Phi_{k,\mathcal{S}}^m$ , with the additional requirement that the sequence of matrices  $\{\tilde{\varphi}_n(\mathbf{0})\}_{n=0}^{\infty}$  is summable.

Again, using orthogonality arguments, we have

$$\begin{aligned} \tilde{\varphi}_{0,1}(\mathbf{u}) &= \frac{1}{\pi} \int_0^{\pi} \mathbf{C}(\theta, \mathbf{u}) d\theta, \\ \tilde{\varphi}_{n,1}(\mathbf{u}) &= \frac{2}{\pi} \int_0^{\pi} \cos(n\theta) \mathbf{C}(\theta, \mathbf{u}) d\theta, \quad \text{for } n \geq 1, \end{aligned} \quad (3.4)$$

whereas for  $d \geq 2$ ,

$$\tilde{\varphi}_{n,d}(\mathbf{u}) = \frac{(2n + d - 1)}{2^{3-d}\pi} \frac{[\Gamma((d-1)/2)]^2}{\Gamma(d-1)} \int_0^{\pi} \mathcal{G}_n^{(d-1)/2}(\cos \theta) (\sin \theta)^{d-1} \mathbf{C}(\theta, \mathbf{u}) d\theta, \quad n \geq 0. \quad (3.5)$$

Following [Berg and Porcu \(2016\)](#), we call the mappings  $\{\tilde{\varphi}_{n,d}(\cdot)\}_{n=0}^{\infty}$  matrix-valued *Schoenberg's functions*. The proof of Theorem 3.1 is deferred to Appendix A for a neater exposition. This characterisation can easily be extended to the case  $\mathbb{S}^d \times G$ , with  $G$  being a locally compact group.

## 3.2 Fundamentals and principles of matrix-valued covariances on spheres

This section puts the basis for a statistical interpretation of matrix-valued space-time covariances. Although some concepts might be discussed on a more general basis, we prefer a presentation on the basis of the class  $\Upsilon_{d,1}^m$ , which covers most of the cases in the literature. Let  $\mathbf{C}$  be an element of the class  $\Upsilon_{d,1}^m$ . Throughout, the diagonal elements  $C_{ii}$  are called marginal covariances, whereas the off-diagonal members  $C_{ij}$ , cross-covariances.

The mapping  $\mathbf{C}$  is called *space-time  $m$ -separable* if there exists two mappings  $\mathbf{C}_S$  and  $\mathbf{C}_T$ , belonging

respectively to  $\Psi_{d,\mathcal{I}}^m$  and  $\Phi_{1,\mathcal{S}}^m$ , such that

$$\mathbf{C}(\theta, u) = \mathbf{C}_{\mathcal{S}}(\theta) \circ \mathbf{C}_{\mathcal{T}}(u), \quad (\theta, u) \in [0, \pi] \times \mathbb{R},$$

where  $\circ$  denotes the Hadamard product.

We call the space-time  $m$ -separability property *complete* if there exists a symmetric, positive definite matrix  $\mathbf{A} \in \mathbb{R}^{m \times m}$ , an element  $\mathbf{C}_{\mathcal{S}}$  of  $\Psi_{d,\mathcal{I}}$ , and an element  $\mathbf{C}_{\mathcal{T}}$  of  $\Phi_{1,\mathcal{S}}$ , such that

$$\mathbf{C}(\theta, u) = \mathbf{A} \mathbf{C}_{\mathcal{S}}(\theta) \mathbf{C}_{\mathcal{T}}(u), \quad (\theta, u) \in [0, \pi] \times \mathbb{R}.$$

We finally define *m-separable* an element of the class  $\Upsilon_{d,1}^m$  for which there exists an element  $\mathbf{C} \in \Upsilon_{d,1}$ , and a matrix  $\mathbf{A}$ , as previously defined, such that

$$\mathbf{C}(\theta, u) = \mathbf{A} \mathbf{C}(\theta, u), \quad (\theta, u) \in [0, \pi] \times \mathbb{R},$$

and of course the special case  $\mathbf{C}(\theta, u) = \mathbf{C}_{\mathcal{S}}(\theta) \mathbf{C}_{\mathcal{T}}(u)$  offers complete space-time  $m$ -separability as previously discussed.

Separability is a very useful property for both modelling and estimation, because the related covariance matrices admit nice factorisations, with consequent alleviation of the computational burdens. At the same time, it is a very unrealistic assumption and the literature has been focussed on how to develop non-separable models.

How to escape from separability is a major deal, and we list some strategies that can be adapted from others proposed in Euclidean spaces. To the knowledge of the authors, none of these strategies have ever been implemented on spheres or spheres across time.

**Linear Models of Coregionalisation** Let  $q$  be a positive integer. Given a collection of matrices  $\mathbf{A}_k$ ,  $k = 1, \dots, q$ , and a collection of elements  $\mathbf{C}_k \in \Upsilon_{d,1}$ , the linear model of coregionalisation has expression

$$\mathbf{C}(\theta, u) = \sum_{k=1}^q \mathbf{A}_k \mathbf{C}_k(\theta, u), \quad (\theta, u) \in [0, \pi] \times \mathbb{R},$$

where a simplification of the type  $\mathbf{C}_k(\theta, u) = \mathbf{C}_{k,\mathcal{S}}(\theta) \mathbf{C}_{\mathcal{T}}(u)$  might be imposed. This model has several drawbacks that have been discussed in [Gneiting et al. \(2010\)](#) as well as in [Daley et al. \(2015\)](#).

**Lagrangian Frameworks** Let  $\mathbf{Z}$  be an  $m$ -variate Gaussian field on the sphere with covariance  $\mathbf{C}_s \in \Psi_{d,\mathcal{I}}^m$ . Let  $\mathcal{R}$  be a random orthogonal matrix with a given probability law. Let

$$\mathbf{Y}(\mathbf{x}, t) := \mathbb{E} \mathbf{Z}(\mathcal{R}^t \mathbf{x}), \quad (\mathbf{x}, t) \in \mathbb{S}^d \times \mathbb{R}.$$

Then,  $\mathbf{Y}$  is a random field with transport effect over the sphere. Clearly,  $\mathbf{Y}$  is not Gaussian and evaluation of the corresponding covariance might be cumbersome, as noted in [Alegría and Porcu \(2016\)](#).

**Multivariate Parametric Adaptation** Let  $p$  be a positive integer. Let  $\mathbf{C}(\cdot, \cdot; \boldsymbol{\lambda})$ , for  $\boldsymbol{\lambda} \in \mathbb{R}^p$ , be a member of the class  $\Upsilon_{d,1}$ . Let  $\boldsymbol{\lambda}_{ij} \in \mathbb{R}^p$  for  $i, j = 1, \dots, p$ . For  $|\rho_{ij}| \leq 1$  and  $\rho_{ii} = 1$ , find the parametric restriction such that  $\mathbf{C} : [0, \pi] \times \mathbb{R}$  defined through

$$C_{ij}(\theta, u) = \rho_{ij} C(\theta, u; \boldsymbol{\lambda}_{ij}), \quad (\theta, u) \in [0, \pi] \times \mathbb{R},$$

is a member of the class  $\Upsilon_{d,1}^m$ . Sometimes the restriction on the parameters can be very severe, in particular when  $m$  is bigger than 2. In Euclidean spaces this strategy has been adopted by [Gneiting et al. \(2010\)](#) and [Apanasovich et al. \(2012\)](#) for the Matérn model, and by [Daley et al. \(2015\)](#) for models with compact support.

**Scale Mixtures** Let  $(\Omega, \mathcal{A}, \mu)$  be a measure space. Let  $\mathbf{C} : [0, \pi] \times \mathbb{R} \times \Omega$  such that

1.  $\mathbf{C}(\cdot, \cdot; \xi) \in \Upsilon_{d,1}^m$  for all  $\xi$  in  $\Omega$ ;
2.  $\mathbf{C}(\theta, u; \cdot) \in L_1(\Omega, \mathcal{A}, \mu)$  for all  $(\theta, u) \in [0, \pi] \times \mathbb{R}$ .

Then,

$$\int_{\Omega} \mathbf{C}(\theta, u; \xi) \mu(d\xi)$$

is still an element of  $\Upsilon_{d,1}^m$ . Of course, simple strategies can be very effective. For instance, one might assume that  $\mathbf{C}(\cdot, \cdot; \xi) = \mathbf{C}(\cdot, \cdot) \mathbf{A}(\xi)$ , with  $\mathbf{C} \in \Upsilon_{d,1}$  and  $\mathbf{A}(\xi) \in \mathbb{R}^{m \times m}$  being a positive definite matrix for any  $\xi \in \Omega$  and such that the hypothesis of integrability above is satisfied.

## 4 Parametric families of space-time cross-covariances of the Gneiting type

This section provides some general results for the construction of multivariate space-time parametric models. The most important feature of the proposed models is that they are non-separable mappings, allowing more flexibility in the study of space-time phenomena. In particular, we focus on covariances with a space-time structure of the Gneiting type (Gneiting, 2002).

Recently, Porcu et al. (2016) have proposed some versions of this model for random fields with spatial locations on the unit sphere. Let us provide a brief review. The mapping  $K : [0, \pi] \times \mathbb{R} \rightarrow \mathbb{R}$  defined as

$$K(\theta, u) = \frac{1}{\{f(\theta)|_{[0, \pi]}\}^{1/2}} g\left(\frac{u^2}{f(\theta)|_{[0, \pi]}}\right), \quad \theta \in [0, \pi], u \in \mathbb{R}, \quad (4.1)$$

is called Gneiting model. Arguments in Porcu et al. (2016) show that  $K$  is a member of the class  $\Upsilon_{d,1}$ , for all  $d \in \mathbb{N}$ , for  $g : [0, \infty) \rightarrow [0, \infty)$  being a completely monotone function, i.e.  $g$  is infinitely differentiable on  $(0, \infty)$  and  $(-1)^n g^{(n)}(t) \geq 0$ , for all  $n \in \mathbb{N}$  and  $t \geq 0$ , and  $f : [0, \infty) \rightarrow (0, \infty)$  is a positive function with completely monotone derivative. Such functions  $f$  are called Bernstein functions (Porcu and Schilling, 2011). Here,  $f(\theta)|_{[0, \pi]}$  denotes the restriction of the mapping  $f$  to the interval  $[0, \pi]$ . Tables 4.1 and 4.2 contain some examples of completely monotone and Bernstein functions, respectively. Some properties about these functions are studied in Porcu and Schilling (2011).

We also consider the modified Gneiting class (Porcu et al., 2016) defined through

$$K(\theta, u) = \frac{1}{f(|u|)^{n+2}} g(\theta f(|u|)), \quad (\theta, u) \in [0, \pi] \times \mathbb{R}, \quad (4.2)$$

where  $n \leq 3$  is a positive integer,  $g : [0, \infty) \rightarrow [0, \infty)$  is a completely monotone function and  $f : [0, \infty) \rightarrow (0, \infty)$  is a strictly increasing and concave function on the positive real line. The mapping (4.2) is a member of the class  $\Upsilon_{2n+1,1}$ .

### 4.1 Multivariate modified Gneiting class on the sphere

In order to illustrate the results following subsequently, a technical Lemma will be useful. We do not provide a proof because it is obtained following the same arguments as in Porcu and Zastavnyi (2011).

**Lemma 4.1.** Let  $m, d$  and  $k$  be strictly positive integers. Let  $(X, \mathcal{B}, \mu)$  be a measure space, for  $X \subset \mathbb{R}$

Table 4.1: Some examples of completely monotone functions. Here,  $K_\nu$  denotes the modified Bessel function of second kind of degree  $\nu$ .

Function	Parameters restriction
$g(t) = \exp(-ct^\gamma)$	$c > 0, 0 < \gamma \leq 1$
$g(t) = (2^{\nu-1}\Gamma(\nu))^{-1}(c\sqrt{t})^\nu K_\nu(c\sqrt{t})$	$c > 0, \nu > 0$
$g(t) = (1 + ct^\gamma)^{-\nu}$	$c > 0, 0 < \gamma \leq 1, \nu > 0$
$g(t) = 2^\nu(\exp(c\sqrt{t}) + \exp(-c\sqrt{t}))^{-\nu}$	$c > 0, \nu > 0$

Table 4.2: Some examples of Bernstein functions.

Function	Parameters restriction
$f(t) = (at^\alpha + 1)^\beta$	$a > 0, 0 < \alpha \leq 1, 0 \leq \beta \leq 1$
$f(t) = \ln(at^\alpha + b)/\ln(b)$	$a > 0, b > 1, 0 < \alpha \leq 1$
$f(t) = (at^\alpha + b)/(b(at^\alpha + 1))$	$a > 0, 0 < b \leq 1, 0 < \alpha \leq 1$

and  $\mathcal{B}$  being the Borel sigma algebra. Let  $\psi : [0, \pi] \times X \rightarrow \mathbb{R}$  and  $\varphi : [0, \infty) \times X \rightarrow \mathbb{R}$  be continuous mappings satisfying

1.  $\psi(\cdot, \xi) \in \Psi_{d, \mathcal{I}}^m$  a.e.  $\xi \in X$ ;
2.  $\psi(\theta, \cdot) \in L_1(X, \mathcal{B}, \mu)$  for any  $\theta \in [0, \pi]$ ;
3.  $\varphi(\cdot, \xi) \in \Phi_{k, \mathcal{I}}^m$  a.e.  $\xi \in X$ ;
4.  $\varphi(u, \cdot) \in L_1(X, \mathcal{B}, \mu)$  for any  $u \in [0, \infty)$ .

Let  $\mathbf{C} : [0, \pi] \times [0, \infty) \rightarrow \mathbb{R}^{m \times m}$  be the mapping defined through

$$\mathbf{C}(\theta, u) = \int_X \psi(\theta, \xi) \varphi(u, \xi) \mu(d\xi), \quad (\theta, u) \in [0, \pi] \times [0, \infty). \quad (4.3)$$

Then,  $\mathbf{C}$  is continuous and bounded. Further,  $\mathbf{C}$  belongs to the class  $\Upsilon_{d, k}^m$ .

We are now able to illustrate the main result within this section. Specifically, we offer a multivariate space-time class generating Gneiting functions with different scale parameters.

**Theorem 4.1.** Let  $m \geq 2$  and  $n \geq 1$  be positive integers. Let  $g : [0, \infty) \rightarrow (0, \infty)$  be a completely monotone function. Consider  $f : [0, \infty) \rightarrow (0, \infty)$  being strictly increasing and concave. Let  $\sigma_i > 0$ ,  $|\rho_{ij}| \leq 1$  and  $c_{ij} > 0$ , for  $i, j = 1, \dots, m$ , be constants yielding the additional condition

$$\sum_{i \neq j} |\rho_{ij}| (c_{ii}/c_{ij})^{n+1} \leq 1. \quad (4.4)$$

Then, the mapping  $\mathbf{C}$ , whose members  $C_{ij} : [0, \pi] \times \mathbb{R} \rightarrow \mathbb{R}$  are defined through

$$C_{ij}(\theta, u) = \frac{\sigma_i \sigma_j \rho_{ij}}{f(|u|)^{n+2}} g\left(\frac{\theta f(|u|)}{c_{ij}}\right), \quad (\theta, u) \in [0, \pi] \times \mathbb{R}, \quad (4.5)$$

belongs to the class  $\Upsilon_{2n+1,1}^m$ . Further, the mapping  $\mathbf{C}$  having members

$$C_{ij}(\theta, u) = \frac{\sigma_i \sigma_j \rho_{ij}}{f(|u|)^{n+2}} \left(1 - \frac{\theta f(|u|)}{c_{ij}}\right)_+^{n+\ell+1}, \quad (\theta, u) \in [0, \pi] \times \mathbb{R}, \quad (4.6)$$

belongs to the class  $\Upsilon_{2n+1,1}^m$  for all  $\ell \geq 0$ , where  $(a)_+ := \max\{0, a\}$

The condition (4.4) comes from the arguments in Daley et al. (2015). The proof of Theorem 4.1 is deferred to Appendix B. Here are some examples.

**Example 4.1.** Taking a completely monotone function  $g$  with the structure of the first entries in Table 4.1, namely  $g(t) = \exp(-t)$ , and the mapping  $f(t) = (1 + c_T t^\alpha)^\beta$ , with  $c_T > 0$  and  $\alpha, \beta \in (0, 1]$ , we can generate from Equation (4.5), and the restrictions in Theorem 4.1, a model of the form

$$C_{ij}(\theta, u) = \frac{\sigma_i \sigma_j \rho_{ij}}{(1 + c_T |u|^\alpha)^{\beta(n+2)}} \exp\left\{-\frac{3\theta(1 + c_T |u|^\alpha)^\beta}{c_{ij}}\right\}, \quad (\theta, u) \in [0, \pi] \times \mathbb{R}. \quad (4.7)$$

**Example 4.2.** Considering  $f$  as in the previous example, we propose the following compactly supported model, generated from Equation (4.6),

$$C_{ij}(\theta, u) = \frac{\sigma_i \sigma_j \rho_{ij}}{(1 + c_T |u|^\alpha)^{\beta(n+2)}} \left(1 - \frac{\theta(1 + c_T |u|^\alpha)^\beta}{c_{ij}}\right)_+^{n+\ell+1}, \quad (\theta, u) \in [0, \pi] \times \mathbb{R}. \quad (4.8)$$

## 4.2 A multivariate Gneiting family based on latent dimension approaches

In this section, we propose a family of space-time matrix-valued covariances obtained from a univariate model. The method used is known as the *latent dimension* approach and has been studied in the Euclidean case by Porcu et al. (2006), Apanasovich and Genton (2010) and Porcu and Zastavnyi (2011). Next, we illustrate the spirit of this approach.

Consider a univariate Gaussian random field defined on the product space  $\mathbb{S}^d \times \mathbb{R} \times \mathbb{R}^k$ , for some positive integers  $d$  and  $k$ , namely  $\{Y(\mathbf{x}, t, \boldsymbol{\xi}) : (\mathbf{x}, t, \boldsymbol{\xi}) \in \mathbb{S}^d \times \mathbb{R} \times \mathbb{R}^k\}$ . Suppose that there exists a mapping  $K : [0, \pi] \times \mathbb{R} \times \mathbb{R}^k \rightarrow \mathbb{R}$  such that  $\text{cov}\{Y(\mathbf{x}, t, \boldsymbol{\xi}_1), Y(\mathbf{y}, s, \boldsymbol{\xi}_2)\} = K(\theta(\mathbf{x}, \mathbf{y}), t-s, \boldsymbol{\xi}_1 - \boldsymbol{\xi}_2)$ , for all  $\mathbf{x}, \mathbf{y} \in \mathbb{S}^d$ ,  $t, s \in \mathbb{R}$  and  $\boldsymbol{\xi}_1, \boldsymbol{\xi}_2 \in \mathbb{R}^k$ , which means that  $K$  is an element of the class  $\Upsilon_{d,k+1}$ . The idea is to



define the components of a space-time  $m$ -variate random field,  $\{\mathbf{Z}(\mathbf{x}, t) = (Z_1(\mathbf{x}, t), \dots, Z_m(\mathbf{x}, t))^\top : (\mathbf{x}, t) \in \mathbb{S}^d \times \mathbb{R}\}$ , as

$$Z_i(\mathbf{x}, t) = Y(\mathbf{x}, t, \boldsymbol{\xi}_i), \quad \mathbf{x} \in \mathbb{S}^d, t \in \mathbb{R}, \boldsymbol{\xi}_i \in \mathbb{R}^k,$$

for  $i = 1, \dots, m$ . Thus, the resulting covariance,  $\mathbf{C}(\cdot) = [C_{ij}(\cdot)]_{i,j=1}^m$ , associated to  $\mathbf{Z}$  is given by

$$C_{ij}(\theta, u) = K(\theta, u, \boldsymbol{\xi}_i - \boldsymbol{\xi}_j), \quad \theta \in [0, \pi], u \in \mathbb{R}.$$

Here, the vectors  $\boldsymbol{\xi}_i$  are handled as additional parameters in the model.

The following two theorems allow to construct different versions of the Gneiting model, using the latent dimension technique.

**Theorem 4.2.** Let  $d$  and  $k$  be two positive integers. Consider  $g$  and  $f$  be completely monotone and Bernstein functions, respectively. Then,

$$K(\theta, \mathbf{v}) = \frac{1}{\{f(\theta)|_{[0,\pi]}\}^{k/2}} g\left(\frac{\|\mathbf{v}\|^2}{f(\theta)|_{[0,\pi]}}\right), \quad (\theta, \mathbf{v}) \in [0, \pi] \times \mathbb{R}^k, \quad (4.9)$$

belongs to the class  $\Upsilon_{d,k}$ , for any positive integer  $d$ .

**Theorem 4.3.** Consider the positive integers  $k$  and  $l$ . Let  $g$  be a completely monotone function and  $f_i$ ,  $i = 1, 2$ , Bernstein functions. Then,

$$K(\theta, \mathbf{u}, \mathbf{v}) = \frac{1}{\{f_2(\theta)|_{[0,\pi]}\}^{l/2} \left\{f_1\left[\frac{\|\mathbf{u}\|^2}{f_2(\theta)|_{[0,\pi]}}\right]\right\}^{k/2}} g\left(\frac{\|\mathbf{v}\|^2}{f_1\left[\frac{\|\mathbf{u}\|^2}{f_2(\theta)|_{[0,\pi]}}\right]}\right), \quad (\theta, \mathbf{u}, \mathbf{v}) \in [0, \pi] \times \mathbb{R}^l \times \mathbb{R}^k, \quad (4.10)$$

belongs to the class  $\Upsilon_{d,k+l}$ , for any positive integer  $d$ .

Note that Theorem 4.2 generalises the Gneiting model (4.1). The proofs of both Theorems 4.2 and 4.3 require technical lemmas and are given in Appendix C and D, respectively.

In order to avoid an excessive number of parameters in the model, we follow the parsimonious strategy in Apanasovich and Genton (2010). Consider  $k = 1$  and the scalars  $\{\xi_1, \dots, \xi_m\}$ . We can consider the parameterisation  $\zeta_{ij} = |\xi_i - \xi_j|^2$ , with  $\zeta_{ij} = \zeta_{ji} > 0$  and  $\zeta_{ii} = 0$ , for all  $i, j = 1, \dots, m$ . In order to model RFs with components having different variances and collocated correlation coefficients, we work with a covariance of the form  $C_{ij}(\theta, u) = \sigma_i \sigma_j \rho_{ij} K(\theta, u, \zeta_{ij})$ , where  $[\sigma_i \sigma_j \rho_{ij}]_{i,j=1}^m$  is a symmetric and positive definite matrix and  $K$  is a mapping as in (4.10).

**Example 4.3.** Let  $f_r(t) = (a_r t^{\alpha_r} + 1)^{\beta_r}$ , for  $r = 1, 2$ , with the corresponding restrictions given in Table 4.2, and  $g(t) = \exp(-t)$ . Then, we obtain the following model

$$C_{ij}(\theta, u) = \frac{\sigma_i \sigma_j \rho_{ij}}{(a_2 \theta^{\alpha_2} + 1)^{\beta_2/2} \left( a_1 \left[ \frac{u^2}{(a_2 \theta^{\alpha_2} + 1)^{\beta_2}} \right]^{\alpha_1} + 1 \right)^{\beta_1/2}} \exp \left\{ - \frac{\zeta_{ij}}{\left( a_1 \left[ \frac{u^2}{(a_2 \theta^{\alpha_2} + 1)^{\beta_2}} \right]^{\alpha_1} + 1 \right)^{\beta_1}} \right\}, \quad (4.11)$$

for  $(\theta, u) \in \mathbb{S}^d \times \mathbb{R}$ .

**Example 4.4.** Another interesting option is to generate a different model through a switch between the second and third arguments of mapping (4.10)

$$C_{ij}(\theta, u) = \frac{\sigma_i \sigma_j \rho_{ij}}{(a_2 \theta^{\alpha_2} + 1)^{\beta_2/2} \left( a_1 \left[ \frac{\zeta_{ij}}{(a_2 \theta^{\alpha_2} + 1)^{\beta_2}} \right]^{\alpha_1} + 1 \right)^{\beta_1/2}} \exp \left\{ - \frac{c_1 u^2}{\left( a_1 \left[ \frac{\zeta_{ij}}{(a_2 \theta^{\alpha_2} + 1)^{\beta_2}} \right]^{\alpha_1} + 1 \right)^{\beta_1}} \right\}, \quad (4.12)$$

for  $(\theta, u) \in \mathbb{S}^d \times \mathbb{R}$ .

On the other hand, a linear model of coregionalisation based on the latent dimension approach can be used to achieve more flexibility. For instance, a model with different marginal covariances can be generated using such an extension. We refer the reader to [Apanasovich and Genton \(2010\)](#) for a more specialised reading about these topics.

## 5 Numerical results

### 5.1 Simulation experiments

The aim of this section is to study some statistical properties of the proposed models. We first focus on some geometrical aspects and then we assess the sample variability of the maximum likelihood estimates of the unknown parameters. We restrict our attention on the bivariate space-time case, with spatial locations on  $\mathbb{S}^2$ , and consider four models. Models 1 and 2 are generated from the modified Gneiting class, whereas Models 3 and 4 are Gneiting models coming from the latent dimension approach. Specifically, we consider:

1. Modified Gneiting covariance defined through Equation (4.7).
2. Modified Gneiting covariance defined through Equation (4.8).
3. Gneiting covariance defined through Equation (4.11).

#### 4. Gneiting covariance defined through Equation (4.12).

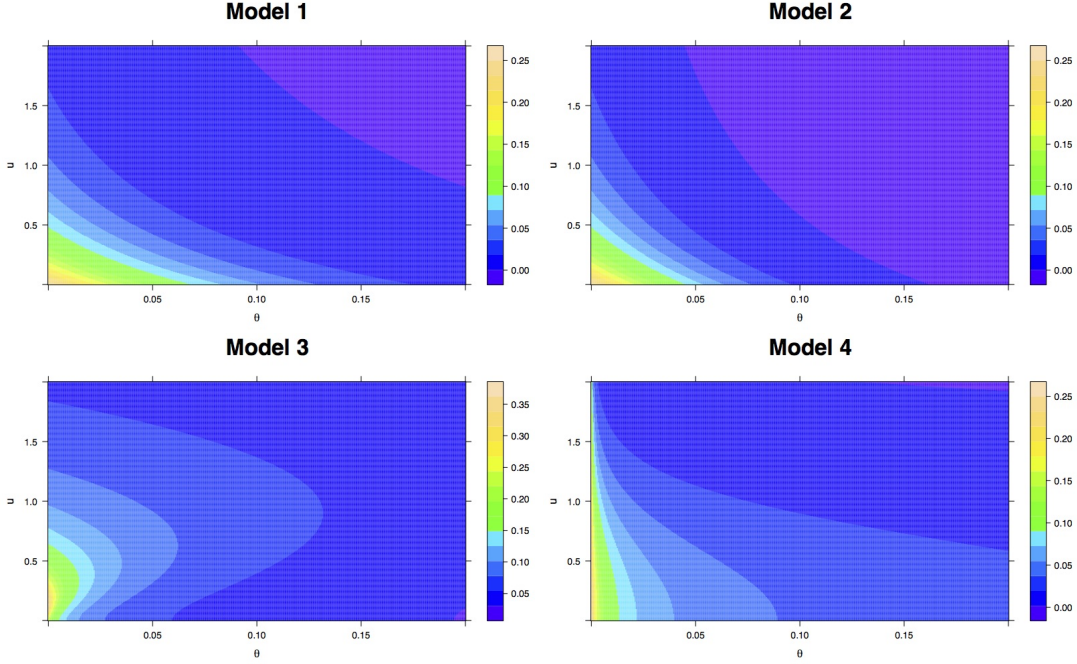
For Models 1 and 2, we fix  $n = 1$  and  $\alpha = \beta = 1$ . In addition, for Model 2 we fix the parameter  $\ell = 1$ . Thus, the parameter vector is given by  $(\sigma_1^2, \sigma_2^2, \rho_{12}, c_{11}, c_{12}, c_{22}, c_T)$ . In the modified Gneiting classes, all parameters have a clear interpretation. Here,  $\sigma_i^2$ , for  $i = 1, 2$ , correspond to the variances of the fields,  $\rho_{12}$  is the collocated correlation coefficient between the components of the field, and  $c_{ij}$ , for  $i, j = 1, 2$ , and  $c_T$  represent spatial and temporal scales, respectively.

On the other hand, for Models 3 and 4, we have kept fixed  $\alpha_i = \beta_i = 1$ , for  $i = 1, 2$ . Also, for Model 3 we have used the re-parameterisations  $a_1 = 400/c_T^2$  and  $a_2 = 400/c_S$ . For Model 4, we fix  $a_1 = 1$  in order to avoid identifiability problems, and we have used the re-parameterisations  $a_2 = 400/c_S$  and  $c_1 = 3/c_T^2$ . The parameter vector for the latent dimension models is given by  $(\sigma_1^2, \sigma_2^2, \rho_{12}, c_S, c_T, \zeta_{12})$ . Here,  $\sigma_i^2$ , for  $i = 1, 2$ , represent the variances, and  $c_S$  and  $c_T$  are spatial and temporal scale parameters, respectively. Note that for Model 3, the collocated correlation between the components of the field is given by  $\rho_{12} \exp\{-\zeta_{12}\}$ . This quantity must belong to the interval  $[-1, 1]$ . Note that  $\rho_{12}$  does not necessarily belong to such interval. Similarly, for Model 4, the collocated correlation between the fields is given by  $\rho_{12}/(\zeta_{12} + 1)^{1/2}$ . Thus, in the latent dimension constructions, the parameter  $\zeta_{12}$  has an impact in the cross scale of the field as well as the correlation between the fields. Also, note that the marginal covariances associated to Model 4 are space-time separable.

Throughout, for Models 1 and 2, we set  $\sigma_1^2 = \sigma_2^2 = 1$ ,  $\rho_{12} = 0.25$ ,  $c_{11} = 0.1$ ,  $c_{22} = 0.3$ ,  $c_{12} = 0.2$  and  $c_T = 0.85$ . For Model 3, we set  $\sigma_1^2 = \sigma_2^2 = \rho_{12} = 1$ ,  $c_S = 1.2$ ,  $c_T = 2$  and  $\zeta_{12} = 1.4$ . For Model 4, we consider  $\sigma_1^2 = \sigma_2^2 = 1$ ,  $\rho_{12} = 0.5$ ,  $c_S = 0.2$ ,  $c_T = 2$  and  $\zeta_{12} = 3$ . With these values, all models have a collocated correlation approximately equal to 0.25 and similar scales.

Figure 5.1 illustrates the contour lines for the space-time cross-covariances,  $C_{12}(\theta, u)$ , with  $(\theta, u)$  in the rectangle  $[0, 0.2] \times [0, 2]$ , associated to Models 1-4. There are remarkable differences between the models. For instance, Model 3 has an interesting behaviour, known as *dimple effect*, which means that for certain predetermined distance  $\theta_0 \in [0, \pi]$ , the covariance is not a monotonically decreasing function of the temporal lag  $u$ . This property has been studied on Euclidean spaces by Kent et al. (2011). They have proved that under certain hypothesis the Gneiting class presents this effect. Kent et al. (2011) argue that in some cases this property can be counterintuitive, but we believe that in many processes influenced by prevailing winds or ocean currents, this effect is consistent. Dimple effects have been studied also for random fields on spheres across time by Alegria and Porcu (2016), for covariances arising from transport phenomena. Figure 5.1 shows that models based on the modified

Figure 5.1: Contour lines of the cross-covariances  $C_{12}(\theta, u)$  for Models 1-4.



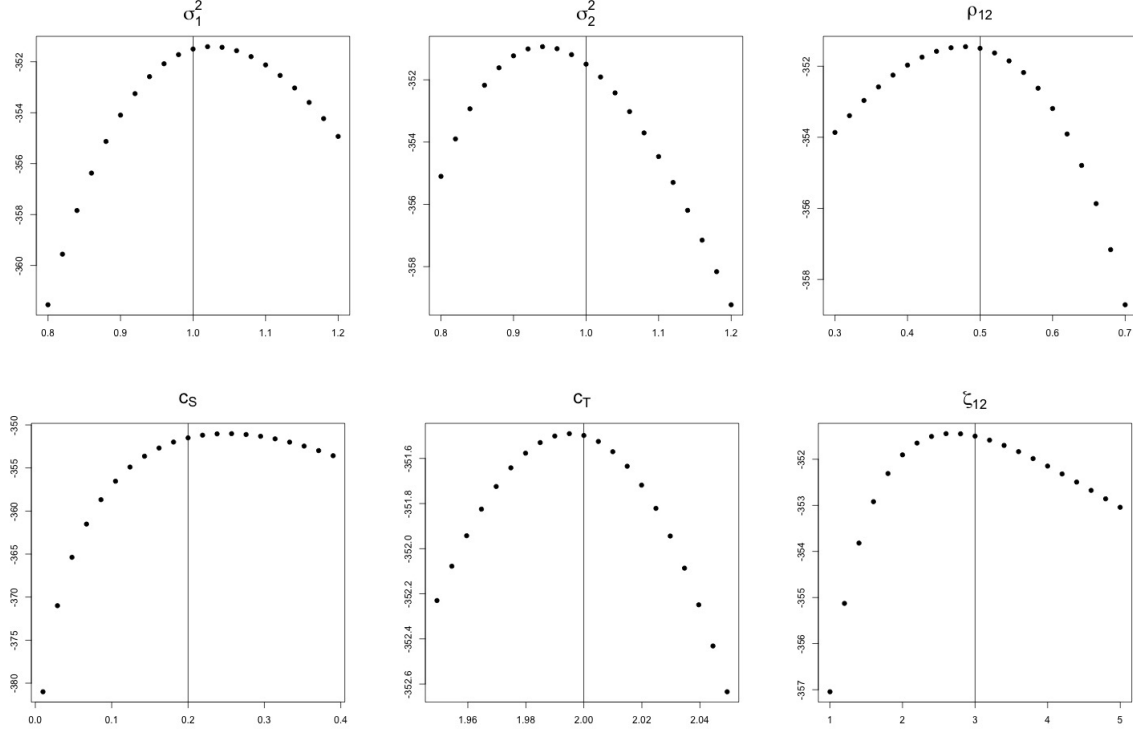
Gneiting class do not have dimples.

Next, we study the maximum likelihood estimates of the parameters. The spatial locations were generated combining 5 equispaced polar and azimuth angles. The resulting spatial grid has 25 sites distributed over the sphere. Moreover, we have considered  $t \in \{1, \dots, 12\}$ . In total, each sample contains 600 observations. We have chosen samples of moderate size to be able to carry out the maximum likelihood estimation.

For Models 1 and 2, Table 5.1 summarises the results of the estimations on the basis of 500 replicates. Similarly, in Table 5.2 we report the results for Models 3 and 4. As expected, the results are quite reasonable for all proposed models. For Models 1 and 2, the cross scale  $c_{12}$  presents greater variability than the other spatial scale parameters. A recurrent strategy reported in the literature is to consider  $c_{12}$  as a function of the marginal scales. In the following section, we show through a data example that such parsimonious strategies provide reasonable results with respect to the full models.

On the other hand, a slight bias can be noticed in the estimation of the temporal scale in Model 3. The parameter  $\zeta_{12}$  has a similar bias in Model 4. [Apanasovich and Genton \(2010\)](#) propose an iterative estimation routine for models based on latent dimensions and suggest some strategies to achieve numerical convergence. Figure 5.2 depicts the profile log likelihoods, with respect to each

Figure 5.2: Profile log likelihoods for a single realisation from Model 4. The vertical lines correspond to the true values.



parameter, for a single realisation from Model 4. For each parameter the curve is unimodal with a well-identified maximum value close to the true value.

Figure 5.3 shows a bivariate realisation, generated from Model 1, over 10000 spatial locations and 2 time instants. The observations were generated using Cholesky decomposition with the following values:  $(\sigma_1^2, \sigma_2^2, \rho_{12}, c_{11}, c_{22}, c_{12}, c_T) = (1, 1, 0.5, 0.5, 1, 0.75, 0.85)$ . The simulated data set can be appreciated through a 360-degrees animation.

## 5.2 Data example: temperatures and pressures

We illustrate the use of the proposed models on a climatological data set. We consider a bivariate space-time data set of surface air temperatures (Variable 1) and atmospheric pressures (Variable 2) obtained from a climate model provided by NCAR (National Center for Atmospheric Research), Boulder, CO, USA. Specifically, the data come from the Community Climate System Model (CCSM4.0) (see [Gent et al., 2011](#)).

Figure 5.3: Bivariate space-time realisation on  $\mathbb{S}^2 \times \{1, 2\}$ , generated from Model 1 through Cholesky decomposition.

Table 5.1: Summary of the maximum likelihood estimates for Models 1 and 2.

Parameter	True	Model 1			Model 2		
		2.5%	Median	97.5%	2.5%	Median	97.5%
$\sigma_1^2$	1	0.8291	1.0043	1.1975	0.8408	0.9949	1.1676
$\sigma_2^2$	1	0.7990	0.9906	1.2121	0.8319	0.9912	1.2025
$\rho_{12}$	0.25	0.0375	0.2523	0.4278	0.0691	0.2624	0.4232
$c_{11}$	0.1	0.0654	0.1018	0.1554	0.0671	0.0998	0.1414
$c_{22}$	0.3	0.2101	0.2971	0.4303	0.2113	0.2991	0.4400
$c_{12}$	0.2	0.0000	0.1894	0.5291	0.0000	0.1898	0.6164
$c_T$	0.85	0.4759	0.8527	3.2529	0.4463	0.8548	2.2941

Table 5.2: Summary of the maximum likelihood estimates for Models 3 and 4.

Parameter	True	Model 3			True	Model 4		
		2.5%	Median	97.5%		2.5%	Median	97.5%
$\sigma_1^2$	1	0.8501	0.9925	1.1950	1	0.8417	0.9920	1.1667
$\sigma_2^2$	1	0.8362	0.9961	1.1995	1	0.8396	0.9927	1.1748
$\rho_{12}$	1	0.0334	1.0876	3.2855	0.5	0.2826	0.5194	1.5827
$c_S$	1.2	0.5862	1.1877	2.6140	0.2	0.0734	0.1953	0.4708
$c_T$	2	0.0605	1.7571	5.2773	2	1.8203	1.9934	2.2269
$\zeta_{12}$	1.4	0.0000	1.4016	4.2164	3	1.1615	3.2055	9.4805

The units are degrees Kelvin for temperatures and Pascal for pressures. The spatial grid is formed by longitudes and latitudes with  $2.5 \times 2.5$  degrees of spatial resolution (10368 grid points). We model planet Earth as a sphere of radius 6378 kilometers. We focus on the month of December between the years 2001 and 2015 (15 time instants).

Since inference is impracticable for such a large data set, we select 343 spatial sites with longitudes in the range  $[-150, 150]$  and latitudes in the range  $[-50, 50]$ . The resulting data set consists of 10290 observations. For each variable and time instant, we use splines to remove the cyclic patterns along longitudes and latitudes. The residuals are approximately Gaussian distributed with zero mean. We re-scale the atmospheric pressures by factor  $(1/200)$  in order to work with both variables in a similar scale. Figure 5.4 shows the residuals of the temperatures and pressures for December 2001. The empirical variances are 28.348 and 3.685, for Variables 1 and 2, respectively. In addition, these variables are strongly negatively correlated. The empirical correlation between the components is  $-0.501$ .

We are interested in showing that in real applications a non-separable model can produce significant improvements with respect to a separable one. For our purposes, we consider a modified Gneiting

Figure 5.4: Residuals of the surface air temperatures (left) and atmospheric pressures (right) for December 2001.



class with increasing level of complexity. Also, we compare the statistical performance of the proposed model with respect to the traditional linear model of coregionalisation (LMC). Specifically, consider the following models:

(A) The modified Gneiting class given in Equation (4.7) and the following special cases:

(A.1) An  $m$ -separable structure under the choice  $c_{11} = c_{22} = c_{12}$ .

(A.2) A parsimonious structure considering  $c_{12} = (c_{11} + c_{22})/2$ .

(A.3) Full model considering all the parameters.

(B) The LMC based on the modified Gneiting class, that is

$$\begin{aligned} C_{11}(\theta, u) &= a_{11}^2 K(\theta, u; c_{S,1}, c_{T,1}) + a_{12}^2 K(\theta, u; c_{S,2}, c_{T,2}) \\ C_{22}(\theta, u) &= a_{21}^2 K(\theta, u; c_{S,1}, c_{T,1}) + a_{22}^2 K(\theta, u; c_{S,2}, c_{T,2}) \\ C_{12}(\theta, u) &= a_{11}a_{21} K(\theta, u; c_{S,1}, c_{T,1}) + a_{12}a_{22} K(\theta, u; c_{S,2}, c_{T,2}), \end{aligned}$$

where

$$K(\theta, u; c_S, c_T) = \frac{1}{(1 + c_T|u|)^3} \exp \left\{ -\frac{3\theta(1 + c_T|u|)}{c_S} \right\}, \quad (\theta, u) \in [0, \pi] \times \mathbb{R}.$$

Here, the vector of parameters is  $(a_{11}, a_{12}, a_{21}, a_{22}, c_{S,1}, c_{S,2}, c_{T,1}, c_{T,2})$ . We focus on the following special cases:

(B.1) A parsimonious structure under the choice  $a_{12} = 0$  and  $c_{T,1} = c_{T,2}$ .



Table 5.3: CL estimates of the parameters for Models (A.1)-(A.3).

	$\hat{\sigma}_1^2$	$\hat{\sigma}_2^2$	$\hat{\rho}_{12}$	$\hat{c}_{11}$	$\hat{c}_{22}$	$\hat{c}_{12}$	$\hat{c}_T$
Model (A.1)	31.325	4.5265	-0.5988	6709.0	6709.0	6709.0	0.0205
Model (A.2)	31.649	4.4707	-0.5985	7676.5	5825.6	6751.1	0.0206
Model (A.3)	31.662	4.4697	-0.5972	7649.7	5828.8	6856.3	0.0206

Table 5.4: CL estimates of the parameters for Models (B.1)-(B.3).

	$\hat{a}_{11}$	$\hat{a}_{21}$	$\hat{a}_{22}$	$\hat{c}_{S,1}$	$\hat{c}_{S,2}$	$\hat{c}_{T,1}$	$\hat{c}_{T,2}$
Model (B.1)	5.6205	-1.2407	1.7129	7499.8	5199.0	0.0206	0.0206
Model (B.2)	5.7459	-1.1665	1.7079	6660.4	6660.4	0.0051	0.0610
Model (B.3)	5.7495	-1.1637	1.7086	6733.5	6396.4	0.0051	0.0604

(B.2) A parsimonious structure under the choice  $a_{12} = 0$  and  $c_{S,1} = c_{S,2}$ .

(B.3) A parsimonious structure under the choice  $a_{12} = 0$ .

Note that for each case we set  $a_{12} = 0$ , since there are no notorious advantages in considering the full case.

Since we are still dealing with a large data set, we estimate the parameters of the model using the pairwise composite likelihood (CL) method developed by [Bevilacqua et al. \(2016\)](#) for multivariate random fields. This method is a likelihood approximation and offers a trade-off between statistical and computational efficiency. We consider only pairs of observations with spatial distance less than 1275.6 kilometers (equivalent to 0.2 on the unit sphere) and temporal distance less than 4 years.

The CL estimates for the Models of type A and B described above are reported in Tables 5.3 and 5.4, respectively. In addition, Table 5.5 contains the log-CL value in the maximum and the number of parameters for each model. Evidently, the non-separable covariances (A.2) and (A.3) exhibit the highest values in the modified Gneiting class. For the LMC, Model (B.3) presents the better performance in terms of the log-CL value. In Figure 5.5, we compare the empirical spatial semi-variograms, for the temporal lags  $|u| = 0$  and  $|u| = 1$ , versus the theoretical models (A.3) and (B.3).

We compare the predictive performance of the covariances through a cross-validation study based on the cokriging predictor. We use a drop-one prediction strategy and quantify the discrepancy between the real and predicted values for each variable through the root mean squared error (RMSE) and the log-score ([Zhang and Wang, 2010](#)). Smaller values of these indicators imply superior predictions.

Table 5.5 displays the results. As expected, the non-separable versions of the modified Gneiting class,

Table 5.5: Comparison of log-CL and cross-validation scores for Models (A.1)-(A.3) and (B.1)-(B.3).

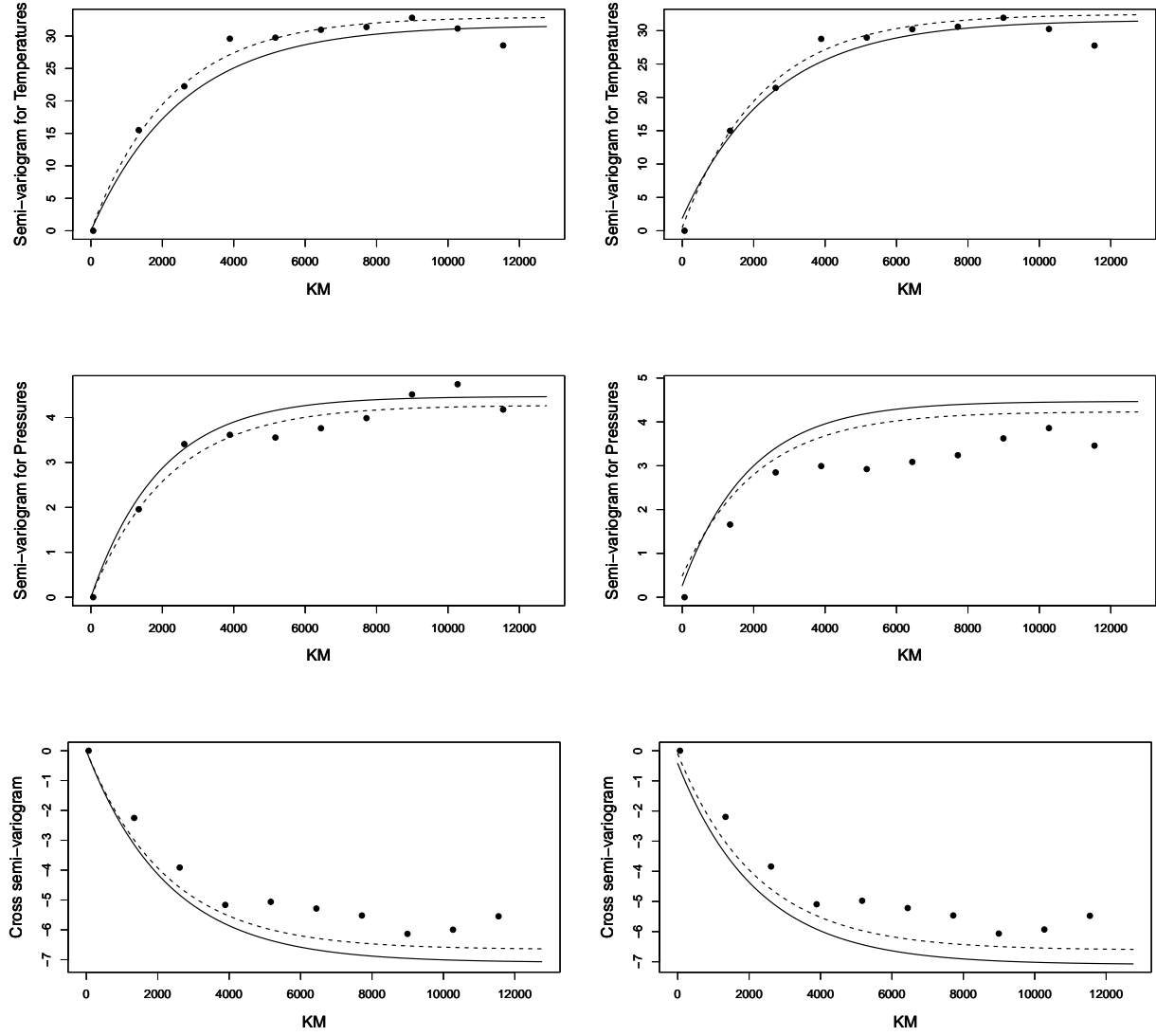
	Num. of parameters	log-CL	RMSE	log-score
Model (A.1)	5	-1211357	0.5806	1.0001
Model (A.2)	6	-1211179	0.5579	0.9270
Model (A.3)	7	-1211179	0.5556	0.9096
Model (B.1)	6	-1211196	0.5429	0.8365
Model (B.2)	6	-1205516	0.5119	0.9435
Model (B.3)	7	-1205513	0.5125	0.9507

(A.2) and (A.3), have better results than their  $m$ -separable counterpart (A.1). If we choose (A.3) instead of (A.1), we have an improvement of 4.3% in terms of the RMSE indicator. Similarly, we have an improvement of 9% in terms of the log-score. For this specific data set, Model (B.2) shows the best results in terms of RMSE, outperforming even Model (B.3). On the other hand, the proposed Models (A.2) and (A.3) outperform in terms of log-score the Models (B.2) and (B.3). In general, a balanced predictive performance between the proposed models and the LMC is observed. A nice property of the modified Gneiting class is that their parameters are physically interpretable. Naturally, the proposed models can be combined to make modelling more flexible.

## 6 Discussion

In the paper we study the characterisation of matrix-valued covariance functions for random fields defined on spheres across time. We have discussed several construction principles that allow to escape from separability. In addition, we have proposed Gneiting type families of cross-covariances and their properties have been illustrated through numerical examples. In particular, we have analysed a bivariate data set of surface air temperatures and atmospheric pressures. The proposed models have shown a good performance using the LMC as a benchmark. We believe that the methodology used to prove our theoretical results can be adapted to find additional flexible classes of matrix-valued covariances and to develop new applications on univariate or multivariate global phenomena evolving temporally.

Figure 5.5: Empirical spatial semi-variograms versus theoretical Models (A.3) (solid line) and (B.3) (dashed line). In the left side we consider the temporal lag as  $|u| = 0$ , whereas in the right side  $|u| = 1$ .



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## Appendices

### A Proof of Theorem 3.1

For a neater exposition, we list some useful results to support our argument:

**Lemma A.0.** Let  $\mathbf{C}$  belong to the class  $\Upsilon_{d,k}^m$  and  $\boldsymbol{\varphi}$  in the class  $\Phi_{d,\mathcal{I}}^m$ . Then,

- (1) For any  $\mathbf{a} \in \mathbb{R}^m$ , we have that the mappings

$$[0, \pi] \times \mathbb{R}^k \ni (\theta, \mathbf{u}) \mapsto \mathbf{C}_{\mathbf{a}}(\theta, \mathbf{u}) := \mathbf{a}^\top \mathbf{C}(\theta, \mathbf{u}) \mathbf{a} \quad (\text{A.1})$$

and

$$\mathbb{R}_+ \ni t \mapsto \boldsymbol{\varphi}_{\mathbf{a}}(t) := \mathbf{a}^\top \boldsymbol{\varphi}(t) \mathbf{a} \quad (\text{A.2})$$

belong to the class  $\Upsilon_{d,k}$  and  $\Phi_{d,\mathcal{I}}$ , respectively.

- (2) Let  $\tilde{\mathbf{C}}$  belong to any of the sets  $\Upsilon_{d,k}$ ,  $\Psi_{d,\mathcal{I}}$  or  $\Phi_{k,\mathcal{S}}$ . Then, the product  $\mathbf{C} \times \tilde{\mathbf{C}}$  belongs to the class  $\Upsilon_{d,k}^m$ .

**Proof of Theorem 3.1** We give a constructive proof. The sufficient part comes from the same arguments as in the proof of Theorem 3.3 in [Berg and Porcu \(2016\)](#). We thus focus on the necessary part. In some occasions we can use the auxiliary notation  $\mathcal{D}_{d,k} := \mathbb{S}^d \times \mathbb{R}^k$ . By Lemma A.0, we have that  $\mathbf{C}_{\mathbf{a}}$ , as defined through Equation (A.1), belongs to the class  $\Upsilon_{d,k}$ . By Lemma 4.3 in [Berg and Porcu \(2016\)](#), we thus have that for any Radon measure  $\mu$  on  $\mathbb{S}^d \times \mathbb{R}^k$  (not necessarily with compact

support, see Remark 4.4), the following expression is non-negative

$$\begin{aligned} \int_{\mathcal{D}_{d,k}} \int_{\mathcal{D}_{d,k}} \mathbf{C}_a(\theta(\mathbf{x}, \mathbf{y}), \mathbf{u} - \mathbf{v}) d\mu(\mathbf{x}, \mathbf{u}) d\mu(\mathbf{y}, \mathbf{v}) &= \int_{\mathcal{D}_{d,k}} \int_{\mathcal{D}_{d,k}} \left( \mathbf{a}^\top \mathbf{C}(\theta(\mathbf{x}, \mathbf{y}), \mathbf{u} - \mathbf{v}) \mathbf{a} \right) d\mu(\mathbf{x}, \mathbf{u}) d\mu(\mathbf{y}, \mathbf{v}) \\ &= \mathbf{a}^\top \left( \int_{\mathcal{D}_{d,k}} \int_{\mathcal{D}_{d,k}} \mathbf{C}(\theta(\mathbf{x}, \mathbf{y}), \mathbf{u} - \mathbf{v}) d\mu(\mathbf{x}, \mathbf{u}) d\mu(\mathbf{y}, \mathbf{v}) \right) \mathbf{a}. \end{aligned}$$

We now pick the product measure  $\mu = \varpi_d \otimes \sigma$ , with  $\varpi$  being the surface measure on the  $d$ -dimensional sphere, and  $\sigma$  a Radon measure on  $\mathbb{R}^k$ . Thus, we can invoke the arguments dealing to Equation (28) of [Berg and Porcu \(2016\)](#) and write

$$\begin{aligned} \mathbf{a}^\top \left( \int_{\mathbb{S}^d \times \mathbb{R}^k} \int_{\mathbb{S}^d \times \mathbb{R}^k} \mathbf{C}(\theta(\mathbf{x}, \mathbf{y}), \mathbf{u} - \mathbf{v}) d\varpi(\mathbf{x}) d\sigma(\mathbf{u}) d\varpi(\mathbf{y}) d\sigma(\mathbf{v}) \right) \mathbf{a} \\ = \mathbf{a}^\top \left( \int_{\mathbb{R}^k \times \mathbb{R}^k} \int_{\mathbb{S}^d} \mathbf{C}(\theta(\boldsymbol{\epsilon}_1, \mathbf{y}), \mathbf{u} - \mathbf{v}) d\varpi(\mathbf{y}) d\sigma(\mathbf{u}) d\sigma(\mathbf{v}) \right) \mathbf{a}, \end{aligned}$$

being non-negative as asserted, and where  $\boldsymbol{\epsilon}_1$  is a unit vector in  $\mathbb{R}^{d+1}$ . Using Lemma A.0(2) and applying the argument above to the function  $\mathbf{C}(\theta, \mathbf{u}) \times \mathcal{G}_n^{(d-1)/2}(\cos \theta)$ , we have that

$$\mathbf{a}^\top \left( \int_{\mathbb{R}^k \times \mathbb{R}^k} \int_{\mathbb{S}^d} \mathbf{C}(\theta(\boldsymbol{\epsilon}_1, \mathbf{y}), \mathbf{u} - \mathbf{v}) \mathcal{G}_n^{(d-1)/2}(\cos \theta(\boldsymbol{\epsilon}_1, \mathbf{y})) d\varpi(\mathbf{y}) d\sigma(\mathbf{u}) d\sigma(\mathbf{v}) \right) \mathbf{a} \quad (\text{A.3})$$

is non-negative for any  $\mathbf{a} \in \mathbb{R}^m$ . Thus, the function

$$\begin{aligned} \tilde{\varphi}_n(\mathbf{u}) &:= \frac{(2n + d - 1)}{2^{3-d}\pi} \frac{[\Gamma((d-1)/2)]^2}{\Gamma(d-1)} \int_{\mathbb{S}^d} \mathbf{C}(\theta(\boldsymbol{\epsilon}_1, \mathbf{y}), \mathbf{u}) \mathcal{G}_n^{(d-1)/2}(\cos \theta(\boldsymbol{\epsilon}_1, \mathbf{y})) d\varpi(\mathbf{y}) \\ &= \frac{(2n + d - 1)}{2^{3-d}\pi} \frac{[\Gamma((d-1)/2)]^2}{\Gamma(d-1)} \int_0^\pi \mathbf{C}(\theta, \mathbf{u}) \mathcal{G}_n^{(d-1)/2}(\cos \theta) (\sin \theta)^{d-1} d\theta, \end{aligned}$$

with  $\mathbf{u} \in \mathbb{R}^k$ , belongs to the class  $\Phi_{k,\mathcal{S}}^m$  for any  $n \in \mathbb{N}$ , since Equation (A.3) holds for all Radon measures with compact support (see [Berg and Porcu, 2016](#)). The rest of the proof follows the steps in [Berg and Porcu \(2016\)](#). In particular, we have that each member  $C_{ij}$  of the function  $\mathbf{C}(\theta(\boldsymbol{\epsilon}_1, \mathbf{x}), \mathbf{u})$  is a continuous mapping, for  $i, j = 1, \dots, m$ . The characterisation of the class  $\Upsilon_{\infty,k}^m$  can be obtained using similar arguments. The proof is completed.

## B Proof of Theorem 4.1

**Proof** Let  $(X, \mathcal{B}, \mu)$  as in Lemma 4.1 and consider  $X = \mathbb{R}_+$  with  $\mu$  the Lebesgue measure. We offer

a proof of the constructive type. Let us define the function  $\psi(\theta, \xi)$  with members  $\psi_{ij}(\cdot, \cdot)$  defined through

$$\psi_{ij}(\theta, \xi) = \sigma_i \sigma_j \rho_{ij} \left(1 - \frac{\theta}{\xi c_{ij}}\right)_+^{n+1}, \quad (\theta, \xi) \in [0, \pi] \times X, \quad i, j = 1, \dots, m,$$

where, as asserted, the constants  $\sigma_i$ ,  $\rho_{ij}$  and  $c_{ij}$  are determined according to condition (4.4). Let us now define the mapping  $(u, \xi) \mapsto \varphi(u, \xi) := \xi^{n+1}(1 - \xi f(u))_+^\ell$ , with  $(u, \xi) \in [0, \infty) \times X$ . It can be verified that both  $\psi$  and  $\varphi$  satisfy requirements 1–4 in Lemma 4.1. In particular, Condition 1 yields thanks to Lemma 3 in Gneiting (2013), as well as Theorem 1 in Daley et al. (2015). Also, arguments in Porcu et al. (2016) show that Condition 3 holds for any  $\ell \geq 1$ . We can now apply Lemma 4.1, so that we have that

$$C_{i,j,n,\ell}(\theta, u) := \int_X \psi(\theta, \xi) \varphi(u, \xi) d\xi, \quad [0, \pi] \times [0, \infty)$$

is a member of the class  $\Upsilon_{2n+1,1}^m$  for any  $\ell \geq 1$ . Pointwise application of an elegant scale mixture argument as in Proposition 1 of Porcu et al. (2016) shows that

$$C_{i,j,n,\ell}(\theta, u) = \mathcal{B}(n+2, \ell+1) \frac{\rho_{ij} \sigma_i \sigma_j}{f(u)^{n+2}} \left(1 - \frac{\theta f(u)}{c_{ij}}\right)_+^{n+\ell+1}, \quad (\theta, u) \in [0, \pi] \times [0, \infty), \quad (\text{B.4})$$

where  $\mathcal{B}$  denotes the Beta function (Abramowitz and Stegun, 1970). Now, standard convergence arguments show that

$$\lim_{\ell \rightarrow \infty} C_{i,j,n,\ell}(\theta/\ell, u) = \mathcal{B}(n+2, \ell+1) \frac{\rho_{ij} \sigma_i \sigma_j}{f(u)^{n+2}} \exp\left(-\frac{\theta f(u)}{c_{ij}}\right), \quad (\theta, u) \in [0, \pi] \times [0, \infty),$$

with the convergence being uniform in any compact set. The proof is then completed in view of Bernstein's theorem (Feller, 1966).

## C Proof of Theorem 4.2

**Lemma C.4.** Let  $C : [0, \pi] \times \mathbb{R}^k \rightarrow \mathbb{R}$  be a continuous, bounded and integrable function, for some positive integer  $k$ . Then  $C \in \Upsilon_{d,k}$ , for  $d \geq 1$ , if and only if the mapping  $\psi_\omega : [0, \pi] \rightarrow \mathbb{R}$  defined as

$$\psi_\omega(\theta) = \frac{1}{(2\pi)^k} \int_{\mathbb{R}^k} \exp\{-i\omega^\top \mathbf{v}\} C(\theta, \mathbf{v}) d\mathbf{v}, \quad \theta \in [0, \pi], \quad (\text{C.5})$$

belongs to the class  $\Psi_{d,\mathcal{I}}$ , for all  $\omega \in \mathbb{R}^k$ .

We do not report the proof of Lemma C.4 since the arguments are the same as in the proof of Lemma

D.5 below. Note that this lemma is a spherical version of the result given by [Cressie and Huang \(1999\)](#).

**Proof of Theorem 4.2** By Lemma C.4, we must show that  $\psi_{\omega}$ , defined through (C.5), belongs to the class  $\Psi_{d,\mathcal{I}}$ , for all  $\omega \in \mathbb{R}^k$ . In fact, we can assume that  $C$  is integrable, since the general case is obtained with the same arguments given by [Gneiting \(2002\)](#). Bernstein's Theorem establishes that  $g$  can be represented as the Laplace transform of a bounded measure  $G$ , then

$$\begin{aligned}\psi_{\omega}(\theta) &= \int_{\mathbb{R}^k} \exp\{-i\omega^\top \mathbf{v}\} \frac{1}{\{f(\theta)|_{[0,\pi]}\}^{k/2}} \int_{[0,\infty)} \exp\left\{-\frac{r\|\mathbf{v}\|^2}{f(\theta)|_{[0,\pi]}}\right\} dG(r) d\mathbf{v} \\ &= \pi^{k/2} \int_{[0,\infty)} \exp\left\{-\frac{\|\omega\|^2}{4r} f(\theta)|_{[0,\pi]}\right\} d\tilde{G}(r),\end{aligned}$$

where the last equality follows from Fubini's Theorem and  $dG(r) = r^{k/2} d\tilde{G}(r)$ . In addition, the composition between a negative exponential and a Bernstein function is completely monotone on the real line ([Feller, 1966](#)). Then, for any  $\omega$  and  $r$ , the mapping  $\theta \mapsto \exp\{-\|\omega\|^2 f(\theta)|_{[0,\pi]}/(4r)\}$  is the restriction of a completely monotone function to the interval  $[0, \pi]$ . Theorem 7 in [Gneiting \(2013\)](#) implies that such mapping, and thus  $\psi_{\omega}$ , belongs to the class  $\Psi_{d,\mathcal{I}}$ , for any  $d \in \mathbb{N}$  and  $\omega \in \mathbb{R}^k$ .

## D Proof of Theorem 4.3

**Lemma D.5.** Let  $C : [0, \pi] \times \mathbb{R}^l \times \mathbb{R}^k \rightarrow \mathbb{R}$  be a continuous, bounded and integrable function, for some positive integers  $l$  and  $k$ . Then,  $C \in \Upsilon_{d,k+l}$ , with  $d \geq 1$ , if and only if the mapping  $C_{\omega} : [0, \pi] \times \mathbb{R}^l \rightarrow \mathbb{R}$  defined as

$$C_{\omega}(\theta, \mathbf{u}) = \frac{1}{(2\pi)^k} \int_{\mathbb{R}^k} \exp\{-i\omega^\top \mathbf{v}\} C(\theta, \mathbf{u}, \mathbf{v}) d\mathbf{v}, \quad (\theta, \mathbf{u}) \in [0, \pi] \times \mathbb{R}^l, \quad (\text{D.6})$$

belongs to the class  $\Upsilon_{d,l}$ , for all  $\omega \in \mathbb{R}^k$ .

**Proof of Lemma D.5** Suppose that  $C \in \Upsilon_{d,k+l}$ , then the characterisation of [Berg and Porcu \(2016\)](#) implies that

$$C(\theta, \mathbf{u}, \mathbf{v}) = \sum_{n=0}^{\infty} \tilde{\varphi}_{n,d}(\mathbf{u}, \mathbf{v}) \frac{\mathcal{G}_n^{(d-1)/2}(\cos \theta)}{\mathcal{G}_n^{(d-1)/2}(1)}, \quad (\text{D.7})$$

where  $\{\tilde{\varphi}_{n,d}(\cdot, \cdot)\}_{n=0}^{\infty}$  is a sequence of functions in  $\Phi_{k+l,\mathcal{S}}$ , with  $\sum_{n=0}^{\infty} \tilde{\varphi}_{n,d}(\mathbf{0}, \mathbf{0}) < \infty$ . Therefore,

$$\begin{aligned}C_{\omega}(\theta, \mathbf{u}) &= \frac{1}{(2\pi)^k} \int_{\mathbb{R}^k} \exp\{-i\omega^\top \mathbf{v}\} \left( \sum_{n=0}^{\infty} \tilde{\varphi}_{n,d}(\mathbf{u}, \mathbf{v}) \frac{\mathcal{G}_n^{(d-1)/2}(\cos \theta)}{\mathcal{G}_n^{(d-1)/2}(1)} \right) d\mathbf{v} \\ &= \sum_{n=0}^{\infty} \left( \frac{1}{(2\pi)^k} \int_{\mathbb{R}^k} \exp\{-i\omega^\top \mathbf{v}\} \tilde{\varphi}_{n,d}(\mathbf{u}, \mathbf{v}) d\mathbf{v} \right) \frac{\mathcal{G}_n^{(d-1)/2}(\cos \theta)}{\mathcal{G}_n^{(d-1)/2}(1)},\end{aligned}$$

where the last step is justified by dominated convergence. We need to prove that for each fixed  $\boldsymbol{\omega} \in \mathbb{R}^k$ , the sequence of functions

$$\mathbf{u} \mapsto \tilde{\lambda}_{n,d}(\mathbf{u}; \boldsymbol{\omega}) := \frac{1}{(2\pi)^k} \int_{\mathbb{R}^k} \exp\{-i\boldsymbol{\omega}^\top \mathbf{v}\} \tilde{\varphi}_{n,d}(\mathbf{u}, \mathbf{v}) d\mathbf{v}, \quad n \geq 0,$$

belongs to the class  $\Phi_{l,\mathcal{S}}$ , a.e.  $\boldsymbol{\omega} \in \mathbb{R}^k$ . In fact, we have that

$$\frac{1}{(2\pi)^l} \int_{\mathbb{R}^l} \exp\{-i\boldsymbol{\tau}^\top \mathbf{u}\} \tilde{\lambda}_{n,d}(\mathbf{u}; \boldsymbol{\omega}) d\mathbf{u} = \frac{1}{(2\pi)^{k+l}} \int_{\mathbb{R}^l} \int_{\mathbb{R}^k} \exp\{-i\boldsymbol{\tau}^\top \mathbf{u} - i\boldsymbol{\omega}^\top \mathbf{v}\} \tilde{\varphi}_{n,d}(\mathbf{u}, \mathbf{v}) d\mathbf{v} d\mathbf{u}. \quad (\text{D.8})$$

Since  $\tilde{\varphi}_{n,d}(\cdot, \cdot)$  belongs to  $\Phi_{k+l,\mathcal{S}}$ , Bochner's Theorem implies that the right side in (D.8) is non-negative everywhere. This implies that  $\tilde{\lambda}_{n,d}(\cdot; \boldsymbol{\omega})$  belongs to the class  $\Phi_{l,\mathcal{S}}$ . Also, direct inspection shows that  $\sum_{n=0}^{\infty} \tilde{\lambda}_{n,d}(\mathbf{0}; \boldsymbol{\omega}) < \infty$ , for all  $\boldsymbol{\omega} \in \mathbb{R}^k$ . The necessary part is completed.

On the other hand, suppose that for each  $\boldsymbol{\omega} \in \mathbb{R}^k$  the function  $C_{\boldsymbol{\omega}}(\theta, \mathbf{u})$  belongs to the class  $\Upsilon_{d,l}$ , then there exists a sequence of mappings  $\{\tilde{\lambda}_{n,d}(\cdot; \boldsymbol{\omega})\}_{n=0}^{\infty}$  in  $\Phi_{l,\mathcal{S}}$  for each  $\boldsymbol{\omega} \in \mathbb{R}^k$ , such that

$$C_{\boldsymbol{\omega}}(\theta, \mathbf{u}) = \sum_{n=0}^{\infty} \tilde{\lambda}_{n,d}(\mathbf{u}; \boldsymbol{\omega}) \frac{\mathcal{G}_n^{(d-1)/2}(\cos \theta)}{\mathcal{G}_n^{(d-1)/2}(1)}.$$

Thus,

$$\begin{aligned} C(\theta, \mathbf{u}, \mathbf{v}) &= \int_{\mathbb{R}^k} \exp\{i\boldsymbol{\omega}^\top \mathbf{v}\} \left( \sum_{n=0}^{\infty} \tilde{\lambda}_{n,d}(\mathbf{u}; \boldsymbol{\omega}) \frac{\mathcal{G}_n^{(d-1)/2}(\cos \theta)}{\mathcal{G}_n^{(d-1)/2}(1)} \right) d\boldsymbol{\omega} \\ &= \sum_{n=0}^{\infty} \left( \int_{\mathbb{R}^k} \exp\{i\boldsymbol{\omega}^\top \mathbf{v}\} \tilde{\lambda}_{n,d}(\mathbf{u}; \boldsymbol{\omega}) d\boldsymbol{\omega} \right) \frac{\mathcal{G}_n^{(d-1)/2}(\cos \theta)}{\mathcal{G}_n^{(d-1)/2}(1)}. \end{aligned}$$

We conclude the proof by invoking again Bochner's Theorem and the result of [Berg and Porcu \(2016\)](#).

**Proof of Theorem 4.3** By Lemma D.5, we must show that (D.6) belongs to the class  $\Upsilon_{d,l}$ , for all  $d \in \mathbb{N}$ . In fact, assuming again that  $C$  is integrable and invoking Bernstein's Theorem we have

$$\begin{aligned} C_{\boldsymbol{\omega}}(\theta, \mathbf{u}) &= \int_{\mathbb{R}^k} \exp\{-i\boldsymbol{\omega}^\top \mathbf{v}\} \frac{1}{\{f_2(\theta)|_{[0,\pi]}\}^{l/2} \left\{ f_1 \left[ \frac{\|\mathbf{u}\|^2}{f_2(\theta)|_{[0,\pi]}} \right] \right\}^{k/2}} \int_{[0,\infty)} \exp \left\{ -\frac{r\|\mathbf{v}\|^2}{f_1 \left[ \frac{\|\mathbf{u}\|^2}{f_2(\theta)|_{[0,\pi]}} \right]} \right\} dG(r) d\mathbf{v} \\ &= \pi^{k/2} \frac{1}{\{f_2(\theta)|_{[0,\pi]}\}^{l/2}} \int_{[0,\infty)} \exp \left\{ -\frac{\|\boldsymbol{\omega}\|^2}{4r} f_1 \left[ \frac{\|\mathbf{u}\|^2}{f_2(\theta)|_{[0,\pi]}} \right] \right\} d\tilde{G}(r), \end{aligned}$$

where the last equality follows from Fubini's Theorem and  $dG(r) = r^{k/2} d\tilde{G}(r)$ . In addition, for any



$\omega$ , the mapping

$$g_{\omega}(\cdot) := \int_{[0,\infty)} \exp \left\{ -\frac{\|\omega\|^2}{4r} f_1(\cdot) \right\} d\tilde{G}(r)$$

is completely monotone (Feller, 1966). Therefore,

$$C_{\omega}(\theta, \mathbf{u}) = \pi^{k/2} \frac{1}{\{f_2(\theta)|_{[0,\pi]}\}^{l/2}} g_{\omega} \left( \frac{\|\mathbf{u}\|^2}{f_2(\theta)|_{[0,\pi]}} \right),$$

and by Theorem 4.2, we have that  $C_{\omega} \in \Upsilon_{d,l}$ , for all  $d \in \mathbb{N}$ .

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